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Notes about the macroscopic fluctuating theory

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Abstract. The macroscopic fluctuating theory developed during the last 30 years is applied to generic systems described by continuum fields $\phi(x,t)$ that evolve by a Langevin equation that locally either conserves or does not conserve the field. This paper aims to review well-known basic concepts and results from a pedagogical point of view by following a general framework in a practical and self-consistent way. From the probability of a path, we study the general properties of the system's stationary state. In particular, we focus on the study of the quasipotential that defines the stationary distribution at the small noise limit. To discriminate between equilibrium and non-equilibrium stationary states, the system's *adjoint dynamics* are defined as the system's time-reversal Markov process. The equilibrium is then defined as the unique stationary state that is dynamically time-reversible, and therefore its adjoint dynamics are equal to those of the original one. This property is confronted with the *macroscopic reversibility* that occurs when the most probable path to create a fluctuation from the stationary state is equal to the time-reversed path that relaxes it. The lack of this symmetry implies a nonequilibrium stationary state; however, the converse is not true. Finally, we extensively study the two-body correlations at the stationary state. We derive some generic properties at various situations, including a discussion about the equivalence of ensembles in nonequilibrium systems.

Keywords: macroscopic fluctuation theory, stationary states, fluctuation phenomena, large deviations in nonequilibrium systems

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Contents

1. Introduction

Nonequilibrium stationary states appear when external agents or boundary conditions drive a system otherwise in equilibrium out of this state by continuously pumping and extracting particles and energy, or simply when a microscopic dynamic breaks some

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spatial symmetry that imposes long-range correlations between their components. In fact, one should recognize that nonequilibrium stationary states are ubiquitous in nature. In contrast, equilibrium states are very scarce and difficult to observe. It is curious that for equilibrium states, we have the thermodynamics and the Boltzmann–Gibbs ensemble theories that permit us to understand and predict the system's macroscopic and mesoscopic (fluctuating) behavior with great success. However, there are no similar general theories for systems at nonequilibrium stationary states. Therefore, it is hard to obtain a general result, derive any prediction from being checked by experiments (numerical or not), or reproduce some observations. After more than two centuries of research, we have just a few (but very relevant from a practical point of view) phenomenological macroscopic relations, such as the Navier–Stokes equation or Fourier law, that are used to describe the behavior of a given fluid or the heat transport, respectively [1]. These depend on constitutive parameters that are obtained by experiments. Moreover, they are based on the assumption that some equilibrium thermodynamic relations apply locally in the system assuming in some sense that the system is not far from equilibrium [2]. Finally, these nonequilibrium descriptions do not include any mesoscopic behavior, and when needed, it is added by hand by taking again as a reference the fluctuations at equilibrium [3]. There has been a lot of effort in recent decades to connect microscopic models with these phenomenological equations [4]. This strategy is fundamental to unveiling the properties of the free parameters (viscosity, thermal conductivity, etc) and the range of such relations' applicability. Nevertheless, this connection has been only partially resolved by the rigorous derivation of hydrodynamic (macroscopic) equations starting from a Boltzmann equation as the microscopic description [5].

From a more fundamental side, in the last 40 years there have been several relevant achievements for systems in nonequilibrium stationary states in understanding the general structure of their stationary attractor in the phase space and the definitions of the invariant measures on it [6]. This Boltzmann-like strategy has permitted us, for instance, to introduce the Sinai–Ruelle–Bowen measures as typical for these systems [7] or to derive the fluctuation theorem [8]. However, from a practical level, we are still far from an instrumental nonequilibrium ensemble theory.

Despite all the efforts mentioned, there are more potential advances for a complete theory of nonequilibrium stationary states by obtaining a deeper understanding of concrete models and systems. There are many techniques, theoretical approaches and/or computer simulations that permit some insight into particular nonequilibrium models in physics, ecology, biophysics etc. Each of the studies presents different characterizations of their nonequilibrium stationary state. Moreover, a set of observables are measured that are assumed to be the optimal ones to describe the particular phenomena. In our opinion, the main problem at present is to find a common theoretical framework flexible enough to permit us to apply it to different situations. This would permit us to compare different approaches, results, or ideas to find the essential properties that characterize nonequilibrium stationary states.

Graham and co-workers took this direction by studying the stationary distribution of a generic white-noise stochastic Langevin equation with finite degrees of freedom in the small noise limit [9]. They found integrability conditions for the quasipotential existence that are the nonequilibrium version of the free energy functionals in thermodynamics.

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Moreover, they analyzed some explicit examples with two degrees of freedom [10] and methods of dealing with stationary states with several attractors [11]. Our paper contains a translation of some of their results. We encourage the reader to look at their seminal work for a deeper understanding of some concepts that we touch lightly on in the spirit of this paper.

In the same line of thought, a promising effort has been made by Bertini *et al* [12] during recent years to develop a mesoscopic theory for diffusive systems that they call *macroscopic fluctuating theory* (MFT). MFT is based on three main assumptions: first, the existence of a well-defined hydrodynamic (macroscopic) description of the system; second, that the fluctuating behavior of the macroscopic variables follows a large deviation principle; and third, that the *fundamental principle* (as they call it) is a generalized *detailed balance condition* that connects the way the system relaxes from a fluctuation to how it was created. All these assumptions are based on previous rigorous results in such one-dimensional microscopic stochastic nonequilibrium models as the boundary-driven symmetric simple exclusion process, the weakly asymmetric exclusion process or the Kipnis–Marchioro–Presutti model (KMP) (see for instance the review by Bertini *et al* [13]). From this solid starting point, MFT intends to obtain the stationary state's general properties in an earnest attempt to understand the behavior of diffusive systems from a theoretical perspective globally. In practice, one may say that MFT is the application of Graham's work to diffusive systems with infinite degrees of freedom or, in other words, systems described by Langevin equations for fields.

In this paper, we extend (in a nonrigorous way) all these seminal works to more general nonequilibrium systems. To do this, we assume as a starting point that our system is defined at the mesoscopic level by a one-component continuum Langevin equation with conserved or nonconserved dynamics and with a local white-noise field that is uncorrelated in time. This set-up allows us to apply many of the MFT concepts to general systems. In section 2, we define the starting equations, some notations and a set of basic definitions and relations. Section 3 is devoted to studying the stationary probability distribution in the small noise limit given by a field's functional, called *quasipotential*. We use the path probability to obtain a Hamilton–Jacobi partial differential equation for the quasipotential. It can be formally solved using the method of characteristics that give us the effective dynamic equations describing the most probable path to create a given fluctuation. This permits us to find some general properties for the quasipotential. In section 4, we introduce the macroscopic reversibility property that is defined when paths to create a fluctuation and the time-reversed deterministic path to relax it coincide. We argue that a macroscopic reversible system has a quasipotential with existing and continuous first and second functional field derivatives. Nevertheless, this property is not enough to guarantee that the system stationary state is an equilibrium state. In section 5, we introduce the fundamental principle that defines the system's *adjoint dynamics* when the time is reversed from a generalized detailed balance condition on paths. Typically the adjoint dynamics are different from the original ones, reflecting the fact that there exists some dissipation that can be related to the existence of nonzero entropy production (see for instance [14]). In this context, the equilibrium is the stationary state of the system when both dynamics coincide. This is consistent with Onsager's idea that the microscopic reversibility extends to the mesoscopic level for systems at

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equilibrium. In section 5, we study the spatial correlations at the stationary state. We obtain the general set of closed equations to study them for the conserved and nonconserved cases. We apply them to some well-known situations to make explicit the power of this theoretical scheme. Moreover, we build the conditions in which conserved and nonconserved situations develop the same quasipotential around the stationary state. This is an attempt to build nonequilibrium dynamical ensembles.

We are convinced that this MFT generalization, although introducing no new paradigms in our basic knowledge of this problem, establishes a theoretical framework that could be useful to many researchers in different fields where these continuous Langevin models are used.

2. Langevin description of mesoscopic systems

We assume that our system, at a hydrodynamic level of description, is completely defined by a unique scalar field $\phi_{\rm D}(x,t) \in IR$ where $x \in \Lambda \subset IR^d$, d is the spatial dimension and t is the time. In this paper, we restrict ourselves to this case for the sake of simplicity, but one can straightforwardly generalize all the results below to systems described by vector fields. The field evolution is the solution of a nonlinear partial differential equation. Along with this work, we consider two separate families of dynamics: the reaction dynamics (RD) that do not conserve the field locally, and the diffusion dynamics (DD) where the field is locally conserved under the evolution:

$$\partial_t \phi_{\rm D}(x,t) = F[\phi_{\rm D}; x, t] \quad \text{(RD case)} \; \partial \phi_{\rm D}(x,t) + \nabla \cdot G[\phi_{\rm D}; x, t] = 0 \quad \text{(DD case)} \quad (1)$$

where F and G are given local functionals of $\phi(x,t)$, $\nabla\phi(x,t)$, etc. Our set of equations are solved typically for given boundary conditions $(\phi_{\rm D}(x,t) = f(x), x \in \partial\Lambda, \forall\, t)$ and an initial state $(\phi_{\rm D}(x,0) = \phi_0(x), x \in \Lambda)$. This determines (hopefully) the solution $\phi_{\rm D}(x,t)$, which is also called the *deterministic or classical solution*. The *stationary state* $\phi^*(x) = \lim_{t\to\infty} \phi_{\rm D}(x,t)$ is the stationary solution of the hydrodynamic equation:

$$F[\phi^*; x] = 0 \quad \text{(RD case) or} \quad \nabla \cdot G[\phi^*; x] = 0 \quad \text{(DD case)}. \quad (2)$$

We assume for simplicity that ϕ^* is unique (in all cases). The stationary state is characterized by the model parameters and the boundary conditions, if any. In a DD with periodic boundary conditions, the initial configuration fixes the system's average density field. The dynamics conserve it and, therefore, it is a parameter that also determines the stationary state. It is also considered that the dynamics are dynamically stable in the sense that all the eigenvalues for the linearized dynamics have a nonzero and negative real part. More precisely, let us expand the hydrodynamic equation around the stationary state: $\phi(x,t) = \phi^*(x) + \epsilon(x,t)$. We then obtain

$$\partial_t \epsilon(x,t) = \int_\Lambda {\rm d}y\, A(x,y)\epsilon(y) + O(\epsilon^2) \quad (3)$$

where

$$A(x,y) = \left.\frac{\delta F[\phi\,; x]}{\delta\phi(y)}\right|_{\phi=\phi^*} \quad \text{(RD case)} \;\; \text{or} \quad A(x,y) = \left.\frac{\delta \nabla G[\phi\,; x]}{\delta\phi(y)}\right|_{\phi=\phi^*} \quad \text{(DD case)}. \quad (4)$$

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Then, we assume that all the eigenvalues λ of the operator A, which are solutions of the equation $\det(A - II\lambda) = 0$, are such that $\mathrm{Re}(\lambda) < 0$. This property guarantees that the stationary state is linearly stable under small perturbations. This is the class of stationary states we are going to study in this paper. Obviously, there are many other stationary states, but they are out of this paper's scope.

The mesoscopic description is built from the hydrodynamics of the system by assuming that the system dynamics are given by a Langevin equation with white noise:

- *Reaction dynamics* (*RD*): the mesoscopic state of the system is described by the local field $\phi(x,t)$ that evolves by:

$$\partial_t \phi(x,t) = F[\phi\,;x,t] + h[\phi\,;x,t]\xi(x,t). \tag{5}$$

- *Diffusion dynamics* (*DD*): the state of the system is completely described by the local field $\phi(x,t)$ and the local current $j(x,t)$. Their evolution is given by the continuity equation:

$$\partial_t \phi(x,t) + \nabla \cdot j(x,t) = 0 \tag{6}$$

  where the current j is chosen to be of the form:

$$j_\alpha(x,t) = G_\alpha[\phi\,;x,t] + \sum_{\beta=1}^{d} \sigma_{\alpha,\beta}[\phi\,;x,t]\psi_\beta(x,t) \quad \alpha = 1,\ldots,d. \tag{7}$$

Here, G and σ are given local functionals of $\phi(x,t)$.

In both cases the boundary conditions and the initial state are the ones given for ϕ_{D}. $\xi(x,t)$ and $\psi_\alpha(x,t)$ are uncorrelated Gaussian random variables:

$$\begin{aligned} \langle \xi(x,t)\rangle &= 0 \\ \langle \xi(x,t)\xi(x',t')\rangle &= \frac{1}{\Omega}\delta(x-x')\delta(t-t') \\ \langle \psi_\alpha(x,t)\rangle &= 0 \\ \langle \psi_\alpha(x,t)\psi_\beta(x',t')\rangle &= \frac{1}{\Omega}\delta_{\alpha,\beta}\delta(x-x')\delta(t-t'). \end{aligned} \tag{8}$$

Observe that, for the sake of simplicity, the correlation matrix for the ψ_α noise is chosen to be proportional to the identity. $\Omega > 0$ is the parameter that controls the time and spatial separation between the mesoscopic and hydrodynamic descriptions. It is assumed that Ω is large enough. This is the so-called *weak noise limit* [9] under which we study the properties of the stationary state in this paper. Observe that the macroscopic case is recovered in the strict limit $\Omega \to \infty$. This is why we refer to it as *MFT*. We see from the Langevin equations (??) that the noise seems to be just a perturbation of the deterministic evolution in this limit. However, we will see that the stationary state's statistics follows a *large deviation principle* that is characterized by a functional of the fields called *quasipotential*. This object, related to the thermodynamic free energy for systems at equilibrium, contains the relevant information of any stationary state. Its study will permit us to see how the structures of many observables change dramatically concerning

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the equilibrium case, even if we are very near to it. In particular, even in the simplest cases, we will see that a nonequilibrium stationary state is related to the existence of long-range correlations and nonlocal and/or singular probability distributions.

The presence of the random variables ξ or ψ_α implies that probabilities characterize the system evolution. At this point, it could be interesting to the reader to consult some classical books about stochastic phenomena for systems that mainly have a finite number of degrees of freedom. Here, the general basic properties of these Langevin equations and many applications to simple illustrative cases can be found [15]. In particular, we are interested in the probability that the system follows a given evolution path ϕ in a time interval. From the Langevin equations, we can explicitly construct such a probability that contains most of the system's interesting physics.

An arbitrary path is defined by the set: $\{\phi\}[t_0, t_1] = (\phi(x,t), x \in \Lambda, t \in [t_0, t_1])$. The probability of this path is just the sum over all sets of random variables that recreate the path multiplied by their probability. For the RD case the path probability is given by:

$$P[\{\phi\}[t_0,t_1]] = \text{cte} \int D\xi \, \exp\left[-\frac{\Omega}{2}\int_{-\infty}^{\infty} \mathrm{d}t \int_\Lambda \mathrm{d}x \, \xi(x,t)^2\right] \cdot \prod_{t\in[t_0,t_1]} \prod_{x\in\Lambda} \delta\left(\partial_t\phi(x,t) - F[\phi\,;x,t] - h[\phi\,;x,t]\xi(x,t)\right) \tag{9}$$

where the constant is found by the normalization of P. We use the integral representation of Dirac's delta to write

$$P[\{\phi\}[t_0,t_1]] = \text{cte} \int D\pi \, \exp\left[-\Omega\int_{t_0}^{t_1} \mathrm{d}t \int_\Lambda \mathrm{d}x \, \pi(x,t)\left(\partial_t\phi(x,t) - F[\phi\,;x,t]\right)\right] \cdot \int D\xi \, \exp\left[\left[-\Omega\int_{t_0}^{t_1} \mathrm{d}t \int_\Lambda \mathrm{d}x \, \left(\frac{1}{2}\xi(x,t)^2 - \pi(x,t)h[\phi\,;x,t]\xi(x,t)\right)\right]\right]. \tag{10}$$

In this way we can explicitly perform the Gaussian integral over the noise variables and obtain

$$P[\{\phi\}[t_0,t_1]] = \text{cte} \int D\pi \, \exp\left[-\Omega\int_{t_0}^{t_1} \mathrm{d}t \left[\int_\Lambda \mathrm{d}x \, \pi(x,t)\partial_t\phi(x,t) - H[\phi(t),\pi(t)]\right]\right] \tag{11}$$

where

$$H[\phi,\pi] = \int_\Lambda \mathrm{d}x \, \pi(x)\left[F[\phi\,;x] + \frac{1}{2}\pi(x)h[\phi\,;x]^2\right]. \tag{12}$$

We could explicitly perform the integral over π, but let us keep this expression for later use.

For the DD case, first we have to give the path probability for the variables that define the state of the system (ϕ, j):

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$$P[\{\phi, j\}\,[t_0, t_1]] = \text{cte} \int D\psi\, \exp\left[-\frac{\Omega}{2}\sum_{\alpha}\int_{-\infty}^{\infty} \mathrm{d}t \int_{\Lambda} \mathrm{d}x\, \psi_\alpha(x,t)^2\right] \cdot$$
$$\prod_{t\in[t_0,t_1]}\prod_{x\in\Lambda}\Bigg[\delta\left(\partial_t\phi(x,t) + \nabla\cdot j(x,t)\right)$$
$$\times \prod_{\alpha}\delta\left(j_\alpha(x,t) - G_\alpha[\phi\,;x,t] - \sum_{\beta}\sigma_{\alpha\beta}[\phi\,;x,t]\psi_\beta(x,t)\right)\Bigg]$$
$$= \text{cte}\, \exp\left[-\frac{\Omega}{2}\int_{t_0}^{t_1}\mathrm{d}t\int_{\Lambda}\mathrm{d}x\,(j(x,t) - G[\phi\,;x,t])\cdot\right.$$
$$\left.\chi^{-1}[\phi\,;x,t]\,(j(x,t) - G[\phi\,;x,t])\right]\cdot$$
$$\prod_{t\in[t_0,t_1]}\prod_{x\in\Lambda}\delta\left(\partial_t\phi(x,t) + \nabla\cdot j(x,t)\right) \tag{13}$$

where $\chi[\phi\,;x,t]$ is a symmetric invertible matrix with components

$$\chi_{\alpha,\beta}[\phi\,;x,t] = \sum_{\gamma=1}^{d}\sigma_{\alpha,\gamma}[\phi\,;x,t]\sigma_{\beta,\gamma}[\phi\,;x,t]. \tag{14}$$

From this expression we can deduce the path probability for ϕ:

$$P[\{\phi\}\,[t_0,t_1]] = \int Dj P[\{\phi,j\}\,[t_0,t_1]]. \tag{15}$$

Again, we introduce the Dirac delta representation; we take $\pi(x,t) = 0\,\forall\, x \in \partial\Lambda$ and we integrate over the j's. After this, we obtain the same expression as equation (11) with

$$H[\phi,\pi] = \int_{\Lambda}\mathrm{d}x\,\nabla\pi(x)\cdot\left[G[\phi\,;x] + \frac{1}{2}\chi[\phi\,;x]\nabla\pi(x)\right]. \tag{16}$$

We are ready to study the stationary distribution at the small noise limit ($\Omega\to\infty$).

3. Stationary state and quasipotential

We assume that the system evolves toward a unique stationary probability distribution $P_{\text{st}}[\phi]$ from almost any initial condition. This stationary distribution could be computed by using the path probability (11) or as the solution of the Fokker–Planck equation (see appendix A) such that $\partial_t P_{\text{st}}[\phi] = 0$. Let us focus on the first strategy because, as we will see, it includes a least-action variational principle that in a more general context is very important in order to select the absolute minimal solution when there are multiple local minimizers of the action (multiple solutions of the stationary Fokker–Planck equation).

The main idea to define the stationary distribution from the path probability is to use the fact that the probability of going from a given starting state to another final

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state in a time interval is just the sum of all the probabilities of every path that connects both states. Therefore, the stationary probability of being at state η is the probability of being at the stationary state ϕ^* times the probability of going from ϕ^* to η in an infinite time interval:

$$P_{st}[\eta] = P_{st}[\phi^*] \int D\phi\, P[\{\phi\}[-\infty, 0]] \prod_{x\in\Lambda} [\delta(\phi(x,0) - \eta(x))\delta(\phi(x,-\infty) - \phi(x)^*)] \quad (17)$$

where $P[\{\phi\}[t_0, t_1]]$ is given by equation (11) and H are obtained from equations (12) or (16) for the RD or DD case, respectively. Except for some elementary models, we do not know how to obtain explicit expressions for $P_{\rm st}[\phi]$. However, we can use the fact that the noise intensity is very small to simplify the problem significantly. When $\Omega \to \infty$ the stationary probability distribution is of the form:

$$P_{st}[\eta] \simeq \exp\left[-\Omega V_0[\eta]\right] \quad (18)$$

where $V_0[\eta]$ is the so-called *quasipotential*. Observe that in the strict limit $\Omega \to \infty$ we should obtain the stationary deterministic solution (2). In other words:

$$P_{st}[\eta] = \prod_{x\in\Lambda} \delta(\eta(x) - \phi^*(x)). \quad (19)$$

This implies that $\phi^*(x)$ is the absolute minimum of the quasipotential:

$$\frac{\delta V_0[\phi^*]}{\delta\phi^*(x)} = 0 \quad \forall\ x \in \Lambda. \quad (20)$$

When $\Omega \to \infty$ the integrals in equation (17) are dominated by the path (ϕ, π) that minimizes the argument of the exponential. This implies:

$$V_0[\eta] = V_0[\phi^*] + \inf_{\phi,\pi} \left\{ \int_{-\infty}^{0} \mathrm{d}t \left[\int_\Lambda \mathrm{d}x\, \pi(x,t)\partial_t\phi(x,t) - H[\phi(t), \pi(t)] \right] \right\} \quad (21)$$

with H given by equations (12) and (16) for the RD and DD systems, respectively. Moreover, $\phi(x, -\infty) = \phi^*(x)$ and $\phi(x, 0) = \eta(x)$. $\pi(x, -\infty) = 0$ and $H[\phi^*, 0] = 0$ by construction. This equation is just the Hamilton variational principle with H being the Hamiltonian [16]. Therefore, the fields $(\bar\pi(x,t), \bar\phi(x,t))$ that minimize the right-hand side of equation (21) are solutions of the Hamilton equations:

$$\begin{aligned} \partial_t\bar\phi(x,t) &= \frac{\delta H\left[\bar\phi(t), \bar\pi(t)\right]}{\delta\bar\pi(x,t)} \\ \partial_t\bar\pi(x,t) &= -\frac{\delta H\left[\bar\phi(t), \bar\pi(t)\right]}{\delta\bar\phi(x,t)} \end{aligned} \quad (22)$$

with the above boundary conditions. Observe that $H[\bar\phi(t), \bar\pi(t)] = 0$ because the Hamiltonian is constant along any trajectory and it is zero at the initial condition. Therefore, equation (21) can be rewritten

$$V_0[\eta] = V_0[\phi^*] + \int_{-\infty}^{0} \mathrm{d}t \int_\Lambda \mathrm{d}x\, \bar\pi(x,t)\partial_t\bar\phi(x,t). \quad (23)$$

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At this point we stress some general issues:

- We can use the path probability to compute the probability to observe a given value of the space and time averages of fields or their functions in a time interval. For sufficiently large times, we can use the large deviation principle to obtain the probability of observing this averaged value and also some relations that are a kind of generalized Green–Kubo formula for systems at nonequilibrium stationary states. This is a very intense research domain that intends to obtain the general properties of these systems by studying such distributions by theoretical approximations and computer simulations (see appendix B).
- We could also use the stationary Fokker–Planck equation, $\partial_t P_{\rm st}[\phi] = 0$ (see appendix A) to perform a Ω^{-1} expansion on it assuming equation (18). At the lowest order of this expansion we obtain the Hamilton–Jacobi equation:

$$H\left[\bar{\phi}, \frac{\delta V_0\left[\bar{\phi}\right]}{\delta \bar{\phi}}\right] = 0 \tag{24}$$

with H given by equations (12) and (16) for the RD and DD systems, respectively. The equation can be solved by the method of characteristics, which implies at the end to solve the same Hamilton equation (22) (see appendix C). That is, $\bar{\pi}(x,t) = \delta V_0[\bar{\phi}]/\delta\bar{\phi}(x,t)\ \forall\ x,t$ and, in particular, $\delta V_0[\phi^*]/\delta\phi^*(x) = 0$ when $t \to -\infty$ as expected.

- We can study equation (22) near the initial condition $(\phi^*, 0)$. The linear approximation is

$$\begin{aligned} \partial_t \epsilon(x,t) &= \int_\Lambda \mathrm{d}y\, [A(x,y)\epsilon(y,t) + B(x,y)\pi(x,t)] \\ \partial_t \pi(x,t) &= -\int_\Lambda \mathrm{d}y\, A(y,x)\pi(y,t) \end{aligned} \tag{25}$$

where $\epsilon(x,t) = \bar{\phi}(x,t) - \phi^*(x)$, $A(x,y) = \delta^2 H[\phi,\pi]/\delta\pi(x)\delta\phi(y)|_{\phi=\phi^*,\pi=0}$. The Lyapunov exponents, λ, of this set of linearized equations are solutions of:

$$\det(A + \lambda \mathbb{I})\det(-A + \lambda\mathbb{I}) = 0. \tag{26}$$

We know that A is a negative defined matrix (see equation (4)) for the RD and DD cases. Therefore, the possible Lyapunov values appear in pairs $(-\lambda, \lambda)$, typical of a Hamiltonian flow. We can define stable and unstable manifolds crossing the stationary point P^* :$(\phi^*, 0)$. All the trajectories that are the solution of equation (22) starting from the stationary point pertain to the unstable manifold, $M_{\rm u}$. This is important from a practical (numerical) point of view if we want to solve the equations of motion: whenever we choose an initial condition P^*, we will stay there forever. Therefore, the right strategy is to reconstruct the unstable manifold around P^* and then take points P_0 of $M_{\rm u}$ as initial conditions for solving the equations of motion (see for instance [17]).

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- The evolution equation (22) are nonlinear and it could be that for a given η there exist, for instance, a couple of pairs $I_1:(\eta,\pi_1)$ and $I_2:(\eta,\pi_2)$ pertaining to the unstable manifold. Therefore, both evolve to the stationary state $(\phi^*,0)$ as $t\to-\infty$ and the quasipotential is:

$$V_0[\eta]=V_0[\phi^*]+\min[A[\eta;c_1],A[\eta;c_2]],\quad A[\eta;c]=\int_c\pi\,\mathrm{d}\phi \tag{27}$$

  where c_1 and c_2 are the paths described by the Hamiltonian trajectories connecting the stationary state with I_1 and I_2 respectively. For the values η_d such that $A[\eta_d;c_1]=A[\eta_d;c_2]$ there are two different associated π_d values depending on how we approach η_d from c_1 or c_2. Therefore, the quasipotential V_0 has a discontinuous first derivative at η_d. This phenomenon is called *Lagrangian transition* and it appears only in systems at nonequilibrium stationary states [9, 18].
- For the RD and DD cases, there is a family of Langevin equations with *a priori* known stationary solutions. For instance, the Langevin equation such that:

$$\begin{aligned}F[\phi;x]&=-\frac{1}{2}h[\phi;x]^2\frac{\delta V[\phi]}{\delta\phi(x)}\quad(\text{RD case})\\ G[\phi;x]&=-\frac{1}{2}\chi[\phi;x]\nabla\frac{\delta V[\phi]}{\delta\phi(x)}\quad(\text{DD case})\end{aligned} \tag{28}$$

  has the quasipotential $V_0[\phi]=V[\phi]$ for any functionals $h[\phi;x]$, $\chi[\phi;x]$ and $V[\phi]$ such that they meet the conditions of stability (4) and behavior at the boundaries $\delta V[\phi]/\delta\phi(x)=0\,\forall\,x\in\partial\Lambda$. These particular cases are relevant because they permit us to build Langevin equations with an *a priori* given stationary state.
- The quasipotential has a relevant dynamic property: it is a Lyapunov functional for $\phi_{\mathrm{D}}(t)$ and $\bar{\phi}(-t)$. That is, it can be proven (see, for instance, [12]) that if

$$S[\phi]=V_0[\phi]-V_0[\phi^*] \tag{29}$$

  then

$$\frac{\mathrm{d}S[\phi_{\mathrm{D}}(t)]}{\mathrm{d}t}\leqslant 0\quad\text{and}\quad\frac{\mathrm{d}S[\bar{\phi}(-t)]}{\mathrm{d}t}\leqslant 0 \tag{30}$$

  where $\phi_{\mathrm{D}}(t)=\{\phi_{\mathrm{D}}(x,t),x\in\Lambda\}$ and $\bar{\phi}(t)=\{\bar{\phi}(x,t),x\in\Lambda\}$ are the solutions of equations (1) and (22) respectively. Moreover,

$$\lim_{t\to\infty}\frac{\mathrm{d}S[\phi_{\mathrm{D}}(t)]}{\mathrm{d}t}=0\quad\text{and}\quad\lim_{t\to\infty}\frac{\mathrm{d}S[\bar{\phi}(-t)]}{\mathrm{d}t}=0. \tag{31}$$

  In other words, the time evolution of the deterministic dynamics $\phi_{\mathrm{D}}(t)$ and the solutions of the so-called *deterministic adjoint dynamics* $\bar{\phi}(-t)$ tend to minimize the quasipotential at all times. Let us prove these properties for the RD case. From the definition of S we write:

$$\frac{\mathrm{d}S[\phi(t)]}{\mathrm{d}t}=\int_\Lambda\mathrm{d}x\,\frac{\delta V_0[\phi(t)]}{\delta\phi(x,t)}\partial_t\phi(x,t). \tag{32}$$

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We know that $\partial_t \phi_{\rm D}(x,t) = F[\phi_{\rm D}; x, t]$ and $\partial_t \bar{\phi}(x,-t) = -F[\bar{\phi}; x, -t] - h[\bar{\phi}; x, -t]^2 \pi(x,-t)$. Therefore:

$$\begin{aligned} \frac{{\rm d}S[\phi_{\rm D}(t)]}{{\rm d}t} &= \int_\Lambda {\rm d}x \, \frac{\delta V_0[\phi_{\rm D}(t)]}{\delta \phi_{\rm D}(x,t)} F[\phi_{\rm D}; x, t] \\ \frac{{\rm d}S[\bar{\phi}(-t)]}{{\rm d}t} &= \int_\Lambda {\rm d}x \, \frac{\delta V_0[\bar{\phi}(-t)]}{\delta \bar{\phi}(x,-t)} \left(-F[\bar{\phi}; x, -t] - h[\bar{\phi}; x, -t]^2 \pi(x,-t) \right). \end{aligned} \tag{33}$$

We now use the Hamilton–Jacobi equation (24) and we obtain the desired result:

$$\begin{aligned} \frac{{\rm d}S[\phi_{\rm D}(t)]}{{\rm d}t} &= -\frac{1}{2} \int_\Lambda {\rm d}x \, h[\phi_{\rm D}; x, t]^2 \left(\frac{\delta V_0[\phi_{\rm D}(t)]}{\delta \phi_{\rm D}(x,t)} \right)^2 \leqslant 0 \\ \frac{{\rm d}S[\bar{\phi}(-t)]}{{\rm d}t} &= -\frac{1}{2} \int_\Lambda {\rm d}x \, h[\bar{\phi}; x, -t]^2 \pi(x,-t)^2 \leqslant 0. \end{aligned} \tag{34}$$

Finally, the unique state in which such derivatives are equal to zero is the stationary state ϕ^*. Therefore, S is a positive defined functional that decreases monotonously with time until it reaches the stationary state. One can perform a very similar computation for the DD case.

- Some different DD models may have the same quasipotential. Let us assume a model with $G[\phi\,; x]$ and $\chi[\phi\,; x]$ having a stationary state ϕ^* and a quasipotential $V_0[\phi]$. Then, any other model with $\bar{G}[\phi; x] = G[\phi; x] + S[x]$ and $\chi[\phi\,; x]$ with $\nabla S(x) = 0 \, \forall \, x \in \Lambda$ has a stationary state $\bar{\phi}^* = \phi^*$ and a quasipotential $\bar{V}_0[\phi] = V_0[\phi]$. This does not imply that they are describing the same physical situation. For instance, their currents $\bar{G}$ and G are different. Therefore, we can conclude with this example that the quasipotential does not always contain all the relevant information about the system stationary state.

It is difficult to explicitly obtain $V_0[\phi]$ from the above definitions. To our knowledge, it has been obtained explicitly only in a few one-dimensional models; for instance, the boundary-driven symmetric exclusion process (SSEP) and the KMP [19, 20]. In both cases, it is found that V_0 presents a nonlocal structure built through an auxiliary field that is a solution of a nonlinear second-order differential equation that includes the boundary conditions. These results illuminate the complex mathematical structure of nonequilibrium stationary states. Finally, let us mention some serious efforts to define perturbative schemes around some known exact stationary state (see, for instance, [21]).

4. Macroscopic reversibility

We have exposed the way to compute the quasipotential V_0 from the Langevin equation that defines the system mesoscopic dynamics. At this point, it seems that there is no formal distinction between a system being in equilibrium or a nonequilibrium stationary state. In any case, we have to build V_0 from our Hamilton variational principle. From this perspective, some fundamental questions arise: how can we know whether a system is in equilibrium or a nonequilibrium stationary state? We already commented

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above on the possibility that V_0 had some nonanalyticities in its domain of definition. This contrasts with the regular behavior we know from the equilibrium ensemble when looking at the corresponding free energy functional. Is, therefore, a systematic nonanalytic behavior the main difference between equilibrium and a nonequilibrium stationary state? Are there any other differences between the two cases? We could try to create a catalog of V_0's by observing the different mathematical properties that can arise from the equations we explicitly obtained. Then, we could argue which ones are compatible with an equilibrium state or not. This mathematical approach could be possible, but we think that trying to characterize equilibrium or nonequilibrium via the structural form of V_0 is not the correct approach. From a physical point of view, there is a clear cut between the two cases, and therefore, the mathematical peculiarities of V_0 are a consequence of it. Therefore we should find an *a priori* property to determine whether or not our system is in an equilibrium state. The key notion here is the behavior of our system under a time-reversal operation. That will clarify most of the above questions and comments.

From a macroscopic point of view, a system (RD or DD) has two deterministic well-defined dynamics: (I) the deterministic evolution equation (1) for which the solution $\phi_{\rm D}(t)$ is the most probable path that the system follows when it *relax* from an arbitrary η initial condition to the stationary state ϕ^*, and (II) the deterministic adjoint dynamics $\bar{\phi}(t)$ that is the solution of the Hamiltonian equations of motion (22) and represents the most probable path that follows a fluctuation from the stationary state ϕ^* to η. We could agree that $\phi_{\rm D}(t)$ and bar $\phi(-t)$ should differ for a system in a nonequilibrium stationary state because the external mechanisms or boundary conditions that create such a state are, by definition, sensitive to the time arrow. Therefore, this property seems to be relevant to discerning between equilibrium and nonequilibrium stationary states. Let us explore it further by defining the concept of macroscopic time reversibility and seeing what the consequences are for a system that has it.

- *Definition*: a system is called macroscopically time-reversible when $\phi_{\rm D}(x,t) = \bar{\phi}(x,-t)$. In other words, the most probable path to create a fluctuation is just the time reversed one to relax the fluctuation using the deterministic dynamic equation.

  Let us first see the consequences of a system being macroscopically time-reversible.

4.1. RD case

Macroscopic time-reversibility implies in this case that

$$\bar{\phi}(x,t) = \phi_{\rm D}(x,-t) \Rightarrow \partial_t \bar{\phi}(x,t) = -F\left[\bar{\phi};x,t\right]. \tag{35}$$

At the same time $\bar{\phi}$ is solution of equation (24):

$$\begin{aligned} \partial_t \bar{\phi}(x,t) &= F\left[\bar{\phi};x,t\right] + h\left[\bar{\phi};x,t\right]^2 \pi\left[x,t\right] \\ \partial_t \pi(x,t) &= -\int_\Lambda {\rm d}y\, \pi(y,t) \left[\frac{\delta F\left[\bar{\phi};y,t\right]}{\delta \bar{\phi}(x,t)} + \frac{1}{2}\frac{\delta h\left[\bar{\phi};y,t\right]^2}{\delta \bar{\phi}(x,t)}\pi(y,t)\right]. \end{aligned} \tag{36}$$

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Equating the first equation from (36) with equation (35), we obtain

$$\partial_t\bar{\phi}(x,t) = F\left[\bar{\phi};x,t\right] + h\left[\bar{\phi};x,t\right]^2\pi(x,t) = -F\left[\bar{\phi};x,t\right] \Rightarrow \pi(x,t) = -\frac{2F\left[\bar{\phi};x,t\right]}{h\left[\bar{\phi};x,t\right]^2}. \quad (37)$$

The $\pi(x,t)$ obtained is also a solution of the second equation of motion in (36). After its substitution we obtain:

$$\int_\Lambda \mathrm{d}y\, F[\phi;y]\left(\frac{\delta}{\delta\phi(y)}\left[\frac{F[\phi;x]}{h[\phi;x]^2}\right] - \frac{\delta}{\delta\phi(x)}\left[\frac{F[\phi;y]}{h[\phi;y]^2}\right]\right) = 0. \quad (38)$$

This is a necessary condition for our system defined by F and h to be *macroscopically time-reversible*.

We also obtain properties of the associated quasipotential V_0 for these systems if we use the fact that $\pi(x,t) = \delta V_0[\bar{\phi}]/\delta\bar{\phi}(x,t)$. Therefore,

$$\frac{\delta V_0[\phi]}{\delta\phi(x)} = -\frac{2F[\phi;x]}{h[\phi;x]^2} \quad (39)$$

$$\int_\Lambda \mathrm{d}y\, F[\phi;y]\left(\frac{\delta^2 V_0[\phi]}{\delta\phi(x)\delta\phi(y)} - \frac{\delta^2 V_0[\phi]}{\delta\phi(y)\delta\phi(x)}\right) = 0. \quad (40)$$

Let us make some remarks:

- For macroscopically time-reversible systems, the first functional derivative of V_0 is *always* a local functional (whenever $F[\phi\,;x]$ is local) independently of the structure of V_0. Moreover, if the system has some boundary conditions then $F[\phi\,;x] = 0\,\forall\, x \in \partial\Lambda$.
- When

$$D[\phi;x,y] \equiv \frac{\delta}{\delta\phi(y)}\left(\frac{F[\phi;x]}{h[\phi;x]^2}\right) \quad (41)$$

  is symmetric: $D[\phi\,;x,y] = D[\phi\,;y,x]$, then condition (38) is fulfilled and the system is macroscopically time-reversible. In this case V_0 is continuous, with continuous first and second functional derivatives. Moreover, $V_0[\phi]$ can be obtained directly by integrating equation (39). Let us reiterate here that in this paper we are considering situations with one unique stationary state. In the case of several stationary states the theory should be generalized when constructing V_0 (see, for instance, [9]), and one may find some nonanalytic behavior on V_0 even in equilibrium when, for instance, there are coexisting phases.
- When $D[\phi\,;x,y] \neq D[\phi\,;y,x]$, the condition given by equation (38) typically fails (in any case one should check that the integral is not zero for any field). Therefore, the system is not macroscopically time-reversible and, as we will see below, it has a nonequilibrium stationary state.
- RD dynamics are built from a twice differential $V[\phi]$ functional, a noise intensity h (see equation (28)) and with boundary conditions (if any) such that $F[\phi\,;x] = 0\,\forall\, x \in \partial\Lambda$ is macroscopically time-reversible and $V_0[\phi] = V[\phi]$. Typical examples of

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these potentials are those of the form:

$$V_0[\phi] = \int_\Lambda \mathrm{d}x\, v[\phi; x] \tag{42}$$

with $v[\phi\,; x]$ having the property

$$\frac{\delta^2 v[\phi; x]}{\delta\phi(v)\delta\phi(z)} = \frac{\delta^2 v[\phi; x]}{\delta\phi(z)\delta\phi(v)} \quad \forall\ v, \quad z \in \Lambda. \tag{43}$$

Then,

$$F[\phi; x] = -\frac{1}{2} h[\phi; x]^2 \int_\Lambda \mathrm{d}y\, \frac{\delta v[\phi; y]}{\delta\phi(x)}. \tag{44}$$

For instance, if we choose the Ginzburg–Landau form:

$$v[\phi; x] = \frac{1}{2}(\nabla\phi)^2 + w(\phi(x)) \tag{45}$$

with $w(\lambda)$ just any one-dimensional function, we find

$$F[\phi; x] = \frac{1}{2} h[\phi; x]^2 \left(\Delta\phi(x) - \left.\frac{\mathrm{d}v(\lambda)}{\mathrm{d}\lambda}\right|_{\lambda=\phi(x)} \right). \tag{46}$$

The corresponding Langevin dynamics are the well-known Hohenberg–Halpering model A [22].

4.2. DD case

A DD system is *macroscopically time-reversible* when the most probable path is a solution of the Hamilton equation (24):

$$\begin{aligned} \partial_t \bar{\phi}(x,t) &= -\nabla \cdot G\left[\bar{\phi}; x, t\right] - \nabla\left(\chi\left[\bar{\phi}; x, t\right] \nabla\pi(x,t)\right) \\ \partial_t \pi(x,t) &= -\int_\Lambda \mathrm{d}y \nabla\pi(y,t) \cdot \left[\frac{\delta G\left[\bar{\phi}; y, t\right]}{\delta\bar{\phi}(x,t)} + \frac{1}{2}\frac{\delta\chi\left[\bar{\phi}; y, t\right]}{\delta\bar{\phi}(x,t)} \nabla\pi(y,t) \right] \end{aligned} \tag{47}$$

with $\bar{\phi}(x, -\infty) = \phi(x)^*$ and $\pi(x, -\infty) = 0$ also solutions of the time-reversed deterministic equation:

$$\partial\bar{\phi}(x,t) = \nabla \cdot G\left[\bar{\phi}; x, t\right]. \tag{48}$$

Therefore, and similarly to the RD case, we obtain two necessary conditions over G and χ

$$\bar{G}[\phi; x] \equiv G[\phi; x] - S(x) = -\frac{1}{2}\chi \cdot \nabla \frac{\delta V_0[\phi]}{\delta\phi(x)}, \quad \nabla \cdot S[x] = 0 \tag{49}$$

where V_0 is independent of $S(x)$, as we commented above, and

$$\int_\Lambda \mathrm{d}y \sum_\gamma \mathcal{D}_\gamma[\phi; y] \left[\left(\partial_{y,\gamma} \frac{\delta}{\delta\phi(y)} \right) \mathcal{D}_\alpha[\phi; x] - \left(\partial_{x,\alpha} \frac{\delta}{\delta\phi(x)} \right) \mathcal{D}_\gamma[\phi; y] \right] = 0 \quad \forall\ \alpha \tag{50}$$

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where

$$\mathcal{D}_\alpha\left[\bar{\phi};x\right]=\sum_\beta \chi^{-1}_{\alpha\beta}\left[\bar{\phi};x\right]\bar{G}_\beta\left[\bar{\phi};x\right]. \tag{51}$$

These equations are very similar to the ones we obtained for the RD case (see equations (37) and (38)) and most of the comments there apply here:

- The conditions about macroscopic time reversibility are defined on $\bar{G}[\phi;x]$. Therefore, $G[\phi;x]+S(x)$ with $\nabla S(x)=0$ is macroscopically time-reversible whenever $G[\phi;x]$ is. Therefore, we may always build DD models with arbitrary net current that are macroscopically time-reversible.
- For macroscopically time-reversible systems, $\nabla\delta V_0/\delta\phi(x)$ is *always* a local functional (whenever $G[\phi;x]$ is local) independently of the structure of V_0.
- Whenever

$$E[\phi;x,y;\alpha,\gamma]=\left(\partial_{x,\alpha}\frac{\delta}{\delta\phi(x)}\right)D_\gamma[\phi;y] \tag{52}$$

  is symmetric: $E[\phi;x,y;\alpha,\gamma]=E[\phi;y,x;\gamma,\alpha]$, then condition (50) is met and the system is macroscopically time-reversible. Moreover, V_0 can be found by integrating equation (49).
- The DD dynamics that are built from a twice differential $V[\phi]$ functional, a noise intensity χ (see equation (28)) and with the appropriate boundary conditions: $G[\phi;x]=0\,\forall\, x\in\partial\Lambda$ is macroscopically time-reversible. In particular, if we choose $V_0[\phi]$ of the form (42) with $v[\phi;x]$ given by equation (45), we obtain:

$$G_\alpha[\phi;x]=\frac{1}{2}\sum_{\beta=1}^{d}\chi_{\alpha\beta}[\phi;x]\partial_\beta\left(\Delta\phi(x)-\left.\frac{\mathrm{d}v(\lambda)}{\mathrm{d}\lambda}\right|_{\lambda=\phi(x)}\right). \tag{53}$$

  This expression corresponds to the Hohenberg–Halpering model B [22].

5. Fundamental principle: adjoint dynamics

Bertini and co-workers defined the adjoint dynamics by extending the large deviation properties of several microscopic stochastic models to diffusive mesoscopic systems [13]. In fact, they generalized Einstein's proposal regarding fluctuations of systems at equilibrium. He connected the probability of having a fluctuation with the minimum reversible work necessary to create it. Their idea is to assume that the probability of any path from an initial stationary state following the system dynamics is equal to the probability of the *time-reversed* path followed by the *adjoint dynamics*. They call this property *the fundamental principle*, and it defines the adjoint dynamics as just the dynamics associated with the time-reversed system. Moreover, they assumed that the adjoint dynamics thus defined follow a mesoscopic equation similar in structure to the original ones. This permitted them to obtain the equations of motion for the fields under the adjoint dynamics' action. Therefore, they could compare both sets of equations of motion to look for properties due to time symmetries. In fact, they saw that this important concept contains

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the essential ingredients to discriminate between systems in nonequilibrium stationary states and systems in equilibrium. We follow these proposals by Bertini and co-workers [13] by assuming that the fundamental principle is valid to our models. Thus, we can obtain the adjoint dynamics for the RD and DD cases.

5.1. RD adjoint dynamics

Let us define the joint probability of a given path from t_0 to t_1 knowing that $\phi[t_0]$ is chosen from the stationary distribution:

$$P\left(\{\phi\}[t_0,t_1]|\phi[t_0]\right) = P_{st}[\phi[t_0]]P[\{\phi\}[t_0,t_1]]. \tag{54}$$

Let us fix a path $\{\phi\}[t_0,t_1]$ and its time-reversed image: $\{\tilde{\phi}\}[-t_1,-t_0]$ where $\tilde{\phi}(x,t) = \phi(x,-t)$. The *fundamental principle* states that

$$P\left(\{\phi\}[t_0,t_1]|\phi[t_0]\right) = P^*\left(\left\{\tilde{\phi}\right\}[-t_1,-t_0]|\tilde{\phi}[-t_1]\right) \tag{55}$$

where P^* is the probability of a path for the adjoint dynamics. We assume now that $\Omega \to \infty$ and using equations (11), (12) and (18) we obtain

$$P(\{\phi\}[t_0,t_1]|\phi[t_0]) \simeq \exp\left[-\Omega R[\{\phi\}[t_0,t_1]]\right] \tag{56}$$

where

$$\begin{aligned} R[\{\phi\}[t_0,t_1]] &= V_0[\phi(t_0)] + \inf_{\pi}\int_{t_0}^{t_1} \mathrm{d}t\left[\int_\Lambda \mathrm{d}x\,\pi(x,t)\partial_t\phi(x,t) - H[\phi(t),\pi(t)]\right] \\ &= V_0[\phi(t_0)] + \int_{t_0}^{t_1}\mathrm{d}t\int_\Lambda \mathrm{d}x\left(\frac{\partial_t\phi(x,t) - F[\phi;x,t]}{2h[\phi;x,t]}\right)^2. \end{aligned} \tag{57}$$

Then, the fundamental principle implies, in this limit,

$$\begin{aligned} &V_0[\phi[t_0]] + \frac{1}{2}\int_{t_0}^{t_1}\mathrm{d}t\int_\Lambda \mathrm{d}x\left(\frac{\partial_t\phi(x,t) - F[\phi;x,t]}{h[\phi;x,t]}\right)^2 \\ &\quad = V_0[\phi[t_1]] + \frac{1}{2}\int_{t_0}^{t_1}\mathrm{d}t\int_\Lambda \mathrm{d}x\left(\frac{\partial_t\phi(x,t) + F^*[\phi;x,t]}{h^*[\phi;x,t]}\right)^2 \end{aligned} \tag{58}$$

for any path $\{\phi\}[t_0,t_1]$, where we have assumed that the adjoint dynamics are defined by the Langevin equation:

$$\partial_t\tilde{\phi}(x,t) = F^*[\tilde{\phi};x,t] + h^*[\tilde{\phi};x,t]\xi(x,t) \tag{59}$$

with ξ being uncorrelated white noise.

Let us show that equation (58) defines the mathematical form of the F^* and h^* functionals. Let us assume that V_0 is differentiable along the path chosen. Then,

$$V_0[\phi[t_1]] - V_0[\phi[t_0]] = \int_{t_0}^{t_1}\mathrm{d}t\,\partial_t V_0[\phi[t]] = \int_{t_0}^{t_1}\mathrm{d}t\int_\Lambda \mathrm{d}x\,\frac{\delta V_0[\phi[t]]}{\delta\phi(x,t)}\partial_t\phi(x,t). \tag{60}$$

Therefore, equation (58) can be written:

$$\int_{t_0}^{t_1} \mathrm{d}t \int_\Lambda \mathrm{d}x \left\{ \frac{1}{2} \left(\frac{1}{h[\phi;x,t]^2} - \frac{1}{h^*[\phi;x,t]^2} \right) (\partial_t \phi(x,t))^2 \right.$$
$$- \left(\frac{F^*[\phi;x,t]}{h^*[\phi;x,t]^2} + \frac{F[\phi;x,t]}{h[\phi;x,t]^2} + \frac{\delta V_0[\phi[t]]}{\delta\phi(x,t)} \right) \partial_t \phi(x,t)$$
$$\left. - \frac{F^*[\phi;x,t]}{2h^*[\phi;x,t]^2} + \frac{F[\phi;x,t]^2}{2h[\phi;x,t]^2} \right\} = 0 \tag{61}$$

for any path and any time interval. Then, we can fix a time t and change paths such that they have arbitrary values for $\partial_t\phi(x,t)$. Therefore, the coefficients of the time derivatives should be equal to zero. Thus:

$$\begin{aligned} &(\partial_t\phi(x,t))^2 : h^*[\phi;x,t] = h[\phi;x,t] \\ &(\partial_t\phi(x,t))^1 : F^*[\phi;x,t] = -F[\phi;x,t] - h[\phi;x,t]^2 \frac{\delta V_0[\phi]}{\delta\phi(x,t)} \\ &(\partial_t\phi(x,t))^0 : \int_\Lambda \mathrm{d}x \, \frac{F^*[\phi;x,t]^2 - F[\phi;x,t]^2}{h[\phi;x,t]^2} = 0 \end{aligned} \tag{62}$$

The first equation indicates that the adjoint dynamics have the same noise intensity as the direct dynamics. The second one shows that its deterministic part is different and depends on the quasipotential. Finally, it can be easily shown that the last equation is just the Hamilton–Jacobi equation (24).

5.2. DD adjoint dynamics

In this case the fundamental principle should be applied to path probabilities for the variables that define the state of the system: (ϕ, j):

$$P\left(\{\phi,j\}\left[t_0,t_1\right]|\phi\left[t_0\right]\right) = P^*\left(\left\{\tilde{\phi},\tilde{\jmath}\right\}\left[-t_1,-t_0\right]|\tilde{\phi}\left[-t_1\right]\right) \tag{63}$$

where

$$P(\{\phi,j\}[t_0,t_1]|\phi[t_0]) = P_{st}[\phi[t_0]]P[\{\phi,j\}[t_0,t_1]]. \tag{64}$$

$P[\{\phi,j\}[t_0,t_1]]$ is defined in equation (13) and the fields associated to the time-reversed path are such: $\tilde{\phi}(x,t) = \phi(x,-t)$, $\tilde{\jmath}(x,t) = -j(x,-t)$. Again, when $\Omega \to \infty$ we obtain

$$V[\phi(t_1)] - V[\phi(t_0)] = \frac{1}{2}\int_{t_0}^{t_1} \mathrm{d}t \int_\Lambda \mathrm{d}x \, \left[(j(x,t) - G[\phi;x,t]) \cdot \chi^{-1}[\phi;x,t] \, (j(x,t) - G[\phi;x,t]) \right.$$
$$\left. - \, (j(x,t) + G^*[\phi;x,t]) \cdot \chi^{*-1}[\phi;x,t] \, (j(x,t) + G^*[\phi;x,t]) \right] \tag{65}$$

where we have assumed that the adjoint dynamics are defined by the Langevin equation

$$\partial_t\tilde{\phi}(x,t) + \nabla \cdot \tilde{\jmath}(x,t) = 0 \tag{66}$$

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with the constitutive equation:

$$\tilde{j}_\alpha(x,t) = G^*_\alpha\left[\tilde{\phi};x,t\right] + \sum_{\beta=1}^{d}\sigma^*_{\alpha,\beta}\left[\tilde{\phi};x,t\right]\psi_\beta(x,t) \quad \alpha = 1,\ldots,d \tag{67}$$

and

$$\chi^*_{\alpha,\beta}\left[\tilde{\phi};x,t\right] = \sum_{\gamma=1}^{d}\sigma^*_{\alpha,\gamma}\left[\tilde{\phi};x,t\right]\sigma^*_{\beta,\gamma}\left[\tilde{\phi};x,t\right]. \tag{68}$$

Relation (65) should hold for any path and, therefore, for any value of $j(x,t)$ at any time. Then,

$$\begin{aligned}
&(j(x,t))^2 : \chi^*\left[\phi;x,t\right] = \chi\left[\phi;x,t\right]\\
&(j(x,t))^1 : G^*\left[\phi;x,t\right] = -G\left[\phi;x,t\right] - \chi\left[\phi;x,t\right]\nabla\frac{\delta V_0\left[\phi\right]}{\delta\phi(x,t)}\\
&(j(x,t))^0 : H\left[\phi,\frac{\delta V_0\left[\phi\right]}{\delta\phi(x,t)}\right] = 0
\end{aligned} \tag{69}$$

where $H[\phi,\pi]$ is given by equation (16).

There are two observations to be made:

- By construction, the quasipotential associated to the adjoint dynamics is the same as that for the original one: $V_0[\phi]$.
- The equation of motion for the deterministic part of the adjoint dynamics (equation (59) for RD or equation (67) for DD without the noise term) is equal to the time-reversed equation of motion that defines the most probable path to create a fluctuation (equation (22)). Therefore: $\tilde{\phi}_{\rm D}(x,t) = \bar{\phi}(x,-t)$. That is, the deterministic path that is followed by the adjoint dynamics to relax an initial configuration ϕ_0 to the stationary state ϕ^* is just the time-reversed most probable path that goes from the stationary state ϕ^* to ϕ_0 by the normal deterministic dynamics.

5.3. Equilibrium vs nonequilibrium

We know that the definition of the equilibrium concept is a very subtle issue. Nevertheless, we could probably agree that at the macroscopic level, equilibrium is a state where the macroscopic properties of a system do not change in time and where there is no flux of any type across it. Moreover, at the mesoscopic level, we could use Gibbs's definition of equilibrium: the state where the probability density function for a configuration is a time-independent solution of Liouville's equation. The definition of equilibrium in the MFT context is difficult because we deal with mesoscopic systems with no *a priori* connection with any underlying mechanical microscopic model. We have a hint from the theory by Onsager and Machlup about fluctuations and relaxation toward the equilibrium of mesoscopic variables [23]. They assumed that the underlying time reversibility of the microscopic equations of motion should appear in the mesoscopic equations to derive their properties near the equilibrium state. Therefore, the mesoscopic dynamics'

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time reversibility should be the essential item that characterizes a system in an equilibrium state. We already know that the *macroscopic time reversibility* property does not discriminate with enough precision equilibrium from nonequilibrium stationary states. For instance, we may always have systems being macroscopically time-reversible with nonzero average currents in a torus. That is typical of nonequilibrium stationary states (see, for instance, the explicit example given by Bertini *et al* in [24]). In contrast, the fundamental principle defined above contains detailed information on the time-reversed mesoscopic dynamics (adjoint dynamics), and it is the natural place to understand the consequences of time-reversal on the RD and DD models (see equations (55) or (63)).

We assume that a system at equilibrium should behave identically under a time-reversal operation. That is, it should follow the same dynamics independently of the arrow time. This happens when the system dynamics follow this proposition:

- *Proposition*: a system is in equilibrium when the adjoint dynamics are equal to the original ones.

This definition of equilibrium applied to the RD and DD systems implies that F and G should be of the form:

$$\begin{aligned} F[\phi;x] &= -\frac{1}{2}h[\phi;x]^2\frac{\delta V_0[\phi]}{\delta\phi(x)} \quad \text{(RD case)} \\ G[\phi;x] &= -\frac{1}{2}\chi[\phi;x]\nabla\frac{\delta V_0[\phi]}{\delta\phi(x)} \quad \text{(DD case)} \end{aligned} \tag{70}$$

where $V_0[\phi]$ is a solution of the Hamilton–Jacobi equation $H[\phi, \delta V_0/\delta\phi] = 0$. Therefore, F and G also have the differential properties that we found for the macroscopically time-reversible systems: $D[\phi\,;x,y] = D[\phi\,;y,x]$ for RD and $E[\phi\,;x,y\,;\alpha,\gamma] = E[\phi\,;y,x\,;\gamma,\alpha]$ for DD, where D is given in (41) and E in (52).

We make some comments:

- In general:

$$\text{Stationary state is in equilibrium} \Rightarrow \text{macroscopically time} - \text{reversible system.} \tag{71}$$

  For systems with RD the reverse implication is true and, therefore, having an equilibrium stationary state is equivalent to being macroscopically time-reversible. For systems with DD the reverse implication is not true because only the macroscopically time-reversible systems with $S(x) = 0$ have an equilibrium stationary state.
- The deterministic current for systems with DD at equilibrium is zero: $G[\phi^*\,;x] = 0$. It is proven (see, for instance, [13]) that for boundary-driven diffusive systems the reverse statement is true and zero deterministic current at the stationary state implies equilibrium. However, this is not true in general. There are systems with zero deterministic current at the stationary state and generic power-law decay of correlations that is typical of nonequilibrium stationary states [25].

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6. Correlations

Another form to get some insight on V_0 is the study of the stationary correlations. There is a direct relation between the quasipotential around the stationary state and the correlations. Let us define

$$Z_0 = \int D\phi P_{st}[\phi] \simeq \int D\phi \, \exp\left[-\Omega V_0[\phi]\right], \quad \Omega \to \infty \tag{72}$$

It can be shown that the two-body correlations on the stationary state are given by

$$C_2(x,y) \equiv \lim_{\Omega\to\infty} \Omega\langle(\phi(x)-\phi^*(x))(\phi(y)-\phi^*(y))\rangle_{st} = -2\frac{\delta \log \bar{Z}_0[V_2]}{\delta V_2(x,y)} \tag{73}$$

where

$$\bar{Z}_0[V_2] = \int D\omega \, \exp\left[-\frac{1}{2}\int_\Lambda \mathrm{d}x \, \mathrm{d}y \, V_2(x,y)\omega(x)\omega(y)\right] \tag{74}$$

and

$$V_2(x,y) = \left.\frac{\delta^2 V_0[\phi]}{\delta\phi(x)\delta\phi(y)}\right|_{\phi=\phi^*}. \tag{75}$$

We have assumed that V_0 can be expanded around its stationary state ϕ^* and we have made the change of variables $\omega(x) = \sqrt{\Omega}(\phi(x)-\phi^*(x))$ in equation (72).

$\bar{Z}_0$ can be explicitly computed because it is a Gaussian-like integral:

$$\bar{Z}_0[V_2] = \mathrm{cte}(\det(V_2))^{-1/2} \tag{76}$$

and after substituting in equation (73) we finally obtain

$$C_2(x,y) = V_2^{-1}(x,y). \tag{77}$$

We can obtain the same result by constructing the quasipotential (23) by solving the Hamilton evolution equation (22) near the stationary state (see appendix D). That is, the two-body correlations are directly related to the curvature of the quasipotential around the stationary state and, apart from their own relevance as measured observables that can be checked by experimentalists, it helps us to understand the mathematical structure of the quasipotential. For instance, if correlations are long-range that would indicate that the relations (70) do not apply because they imply local behavior of correlations.

From now on, we are going to focus on stationary two-body correlations. In order to find a self-consistent way to compute C_2, we need to go through a more elaborate scheme [13, 15, 21].

Let us first define the *generating functional*:

$$Z[b] = Z[0] \int D\phi \, P_{st}[\phi] \exp\left[\Omega \int_\Lambda \mathrm{d}x \, b(x)\phi(x)\right] \tag{78}$$

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where $b(x)$ is a kind of auxiliary external field. We know from this expression that the n-body correlations at the stationary state (at zero field) are given by

$$\langle \phi(x_1) \dots \phi(x_n) \rangle_{st} = \frac{1}{\Omega^n Z[0]} \frac{\delta^n Z[b]}{\delta b(x_1) \dots \delta b(x_n)} \bigg|_{b=0}. \tag{79}$$

The truncated n-body correlations are defined by:

$$\langle \phi(x_1) \dots \phi(x_n) \rangle^c_{st} = \frac{1}{\Omega^n} \frac{\delta^n W[b]}{\delta b(x_1) \dots \delta b(x_n)} \bigg|_{b=0} \tag{80}$$

where $W[b] = \ln Z[b]$,

$$\langle \phi(x_1) \dots \phi(x_n) \rangle^c_{st} = \langle (\phi(x_1) - \langle \phi(x_1) \rangle_{st}) \dots (\phi(x_n) - \langle \phi(x_n) \rangle_{st}) \rangle_{st} \quad n > 1 \tag{81}$$

and $\langle \phi(x) \rangle^c_{st} = \langle \phi(x) \rangle_{st}$.

We know that $P_{\rm st}[\phi] \propto \exp[-\Omega V_0[\phi]]$ when $\Omega \to \infty$. Then, the generating functional (78) can be written:

$$Z[b] \propto \int D\phi \, \exp[-\Omega \mathcal{F}[\phi, b]], \quad \mathcal{F}[\phi, b] = V_0[\phi] - \int_\Lambda \mathrm{d}x \, b(x)\phi(x). \tag{82}$$

Let us define $\phi^*[b]$ as the field that minimizes $\mathcal{F}$ and let us assume that $\mathcal{F}[\phi, b]$ is differentiable on ϕ's around $\phi^*[b]$; then,

$$\mathcal{F}[\phi, b] = \mathcal{F}[\phi^*[b]] + \frac{1}{2} \int_\Lambda \mathrm{d}x \, \mathrm{d}y \frac{\delta^2 \mathcal{F}[\phi, b]}{\delta\phi(x)\phi(y)} \bigg|_{\phi=\phi^*[b]} (\phi(x) - \phi^*[x; b])(\phi(y) - \phi^*[y; b]) + \cdots \tag{83}$$

where $\phi^*[b]$ is a solution of

$$\frac{\delta \mathcal{F}[\phi, b]}{\delta\phi(x)} \bigg|_{\phi=\phi^*[b]} = 0 \quad \Rightarrow \quad \frac{\delta V_0[\phi]}{\delta\phi(x)} \bigg|_{\phi=\phi^*[b]} = b(x). \tag{84}$$

We observe that $\phi^*[0] = \phi^*$, the minimum of $V_0[\phi]$.

Therefore, we obtain an expansion of the generating functional:

$$Z[b] \propto \mathrm{e}^{-\Omega \mathcal{F}[\phi^*[b], b]} \int D\omega \, \exp\left[-\frac{1}{2} \int_\Lambda \mathrm{d}x \, \mathrm{d}y \frac{\delta^2 V_0[\phi]}{\delta\phi(x)\phi(y)} \bigg|_{\phi=\phi^*[b]} \omega(x)\omega(y) + O(\Omega^{-1/2}) \right] \tag{85}$$

where $w(x) = \sqrt{\Omega}(\phi(x) - \phi^*[x; b])$. We see that this expression has some meaning whenever V_0 is differentiable and convex around $\phi^*[b]$. Convexity also guarantees that there is a one-to-one relation between b and $\phi^*[b]$. It may also be shown that

$$\frac{\delta \mathcal{F}[\phi^*[b], b]}{\delta b(x)} = -\phi^*[x; b]. \tag{86}$$

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That is, $\mathcal{F}[b] \equiv \mathcal{F}[\phi^*[b], b]$ is the Legendre transform of $V_0[\phi]$. We can now relate $\mathcal{F}$ with the correlations:

$$W[b] = -\Omega \mathcal{F}[\phi^*[b]] + O(\Omega^0) \tag{87}$$

and

$$\lim_{\Omega\to\infty} \Omega^{n-1} \langle \phi(x_1) \dots \phi(x_n) \rangle^c_{st} = -\left. \frac{\delta^n \mathcal{F}[\phi^*[b]]}{\delta b(x_1) \dots \delta b(x_n)} \right|_{b=0} \equiv C_n(x_1, \dots, x_n) \tag{88}$$

where $\langle \phi(x) \rangle^c_{st} = \langle \phi(x) \rangle_{st} = \phi^*(x) = \phi^*[x; 0]$.

At this point we can use a trick to build a set of closed equations for the correlation functions. The Hamilton–Jacobi equation applied to $\phi^*(x\,; b)$ is given by:

$$H \left[\phi^*[b], \left. \frac{\delta V_0[\phi]}{\delta \phi} \right|_{\phi=\phi^*[b]} \right] = H\left[\phi^*[b], b\right] = 0 \tag{89}$$

where $H[\phi, \pi]$ is given by equations (12) and (16) for the RD and DD, respectively. We know that

$$\phi^*[x; b] = \phi^*(x) + \int_\Lambda \mathrm{d}y\, C_2(x, y) b(y) + O(b^2). \tag{90}$$

Then, we can implement a perturbative expansion on H around $b = 0$:

$$\int_\Lambda \mathrm{d}x\, \mathrm{d}y\, b(x) b(y) \left[\frac{\delta^2 H[\phi, \pi]}{\delta\pi(x)\delta\pi(y)}|_{\substack{\phi=\phi^* \\ \pi=0}} + \int_\Lambda \mathrm{d}z \left[\frac{\delta^2 H[\phi, \pi]}{\delta\phi(x)\delta\pi(z)}|_{\substack{\phi=\phi^* \\ \pi=0}} C_2(z, y) + \left. \frac{\delta^2 H[\phi, \pi]}{\delta\phi(y)\delta\pi(z)} \right|_{\substack{\phi=\phi^* \\ \pi=0}} C_2(z, x) \right] \right] = O(b^3) \quad \forall\ b \tag{91}$$

where we have used the facts that H is a second-order polynomial in π and that $H[\phi^*, 0] = 0$. Therefore,

$$\int_\Lambda \mathrm{d}z \left[\left. \frac{\delta^2 H[\phi, \pi]}{\delta\phi(x)\delta\pi(z)} \right|_{\substack{\phi=\phi^* \\ \pi=0}} C_2(z, y) + \left. \frac{\delta^2 H[\phi, \pi]}{\delta\phi(y)\delta\pi(z)} \right|_{\substack{\phi=\phi^* \\ \pi=0}} C_2(z, x) \right] = -\left. \frac{\delta^2 H[\phi, \pi]}{\delta\pi(x)\delta\pi(y)} \right|_{\substack{\phi=\phi^* \\ \pi=0}}. \tag{92}$$

Let us explicitly apply equation (92) to the RD and DD cases.

6.1. RD case

We substitute H from equation (12) into (92) and we obtain:

$$\int_\Lambda \mathrm{d}z \left[B(x, z) \bar{C}(z, y) + B(y, z) \bar{C}(z, x) \right] = -\delta(x - y) \tag{93}$$

where

$$C_2(x, y) = h[\phi^*; x] h[\phi^*; y] \bar{C}(x, y) \tag{94}$$

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and

$$B(x,y) = \frac{h[\phi^*;y]}{h[\phi^*;x]} \frac{\delta F[\phi;x]}{\delta \phi(y)}|_{\phi=\phi^*}. \tag{95}$$

Observe that B may be nonsymmetric on its arguments, while $\bar{C}$ is symmetric by construction. We can think of this equation as a representation of the linear operator equation:

$$B\bar{C} + \bar{C}B = -I \tag{96}$$

with I the identity operator. The formal solution can be found by using the fact that $\partial/\partial\alpha\, \mathrm{e}^{\alpha B} = B\, \mathrm{e}^{\alpha B}$. Then,

$$\frac{\partial}{\partial \alpha}\left[\mathrm{e}^{\alpha B}\bar{C}\,\mathrm{e}^{\alpha B^T}\right] = -\mathrm{e}^{\alpha B}\,\mathrm{e}^{\alpha B^T} \Rightarrow \bar{C} = \int_0^\infty \mathrm{d}\alpha\, \mathrm{e}^{\alpha B}\,\mathrm{e}^{\alpha B^T} \tag{97}$$

where we have assumed that B is negative defined. A simple representation of this equation can be obtained in the case in which B is *diagonalizable*; in other words, when we can apply to B some spectral theorem. Let $v(x\,;\lambda_n)$ and $w(x\,;\lambda_n)$ be the set of *right* and *left* eigenvectors of B with eigenvalues λ_n and λ_n^* (complex conjugate of λ_n) respectively:

$$\begin{aligned} &\int_\Lambda \mathrm{d}y\, B(x,y)v(y;\lambda_n) = \lambda_n v(x;\lambda_n) \\ &\int_\Lambda \mathrm{d}y\, B(y,x)w(y;\lambda_n) = \lambda_n^* w(x;\lambda_n). \end{aligned} \tag{98}$$

The eigenvalues may have real or complex values but, because B is real valued, they appear in pairs when they are complex: $(\lambda, v(x\,;\lambda))$, $(\lambda^*, v(x\,;\lambda^*) = v(x\,;\lambda)^*)$. We assume that each set forms a complete basis on the functional space and that they follow the orthogonality conditions:

$$\begin{aligned} &\int_\Lambda \mathrm{d}x\, w(x;\lambda_n)^* v(x;\lambda_m) = \delta_{n,m} \\ &\sum_n w(x;\lambda_n)^* v(y;\lambda_n) = \delta(x-y). \end{aligned} \tag{99}$$

Finally, solution (97) can be written:

$$\bar{C}(x,y) = -\sum_{n,m} \frac{v(x;\lambda_n)v(y;\lambda_m)}{\lambda_n + \lambda_m} \int_\Lambda \mathrm{d}z\, \bar{w}(z;\lambda_n)\bar{w}(z;\lambda_m). \tag{100}$$

We see that the solution is symmetric, $\bar{C}(x,y) = \bar{C}(y,x)$, and real, $\bar{C}(x,y)^* = \bar{C}(x,y)$, due to the pairing property of the eigenvalues.

Solution (100) can be further simplified if B is symmetric: $B(x,y) = B(y,x)$. In this case the right and left eigenvalues and eigenvectors coincide; all of them are real and

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the eigenvectors form an orthonormal base on the functional space. Therefore,

$$\bar{C}(x,y) = -\frac{1}{2}\sum_n \frac{1}{\lambda_n} v(x;\lambda_n)v(y;\lambda_n) = -\frac{1}{2}B^{-1}(x,y) \tag{101}$$

where

$$\int_\Lambda \mathrm{d}z\, B(x,z)B^{-1}(z,y) = \delta(x-y). \tag{102}$$

As an example, let us apply these results to small deviations from equilibrium. Let us assume that a system at equilibrium has a given quasipotential $V_0[\phi]$ and its Langevin dynamics are defined by the pair (F,h) where we know that F is of the form (70). Therefore, the correlations are given by equation (77): $C_2(x,y) = V_2^{-1}(x,y)$. This reference system is now forced to slightly deviate from the equilibrium by imposing a perturbation in the F term. That is, the Langevin equation for the new system is composed of the pair $(\tilde{F},h)$ where

$$\tilde{F}[\phi;x] = -\frac{1}{2}h[\phi;x]^2\left[1+\epsilon g[\phi;x]\right]\frac{\delta V_0[\phi]}{\delta\phi(x)}. \tag{103}$$

$V_0[\phi]$, $g[\phi\,;x]$ and $h[\phi\,;x]$ are given functionals and ϵ can be used as a perturbative parameter. This change does not modify the system stationary solution ϕ^* for any ϵ: $\tilde{F}[\phi^*;x] = 0\,\forall\,\epsilon$. Therefore, the quasipotential $V_\epsilon[\phi]$ associated to the dynamics (103) always has the same extremal state: $\delta V_\epsilon[\phi]/\delta\phi(x)|_{\phi=\phi^*} = 0$ for any ϵ value.

To compute the correlations for the dynamics defined in equation (103), we need to construct the matrix B given by equation (95):

$$B(x,y) = (1+\epsilon g[\phi^*;x])\tilde{B}(x,y), \qquad \tilde{B}(x,y) = -\frac{1}{2}h[\phi^*;x]h[\phi^*;y]\frac{\delta^2\tilde{V}[\phi]}{\delta\phi(x)\delta\phi(y)}|_{\phi=\phi^*} \tag{104}$$

and the equation for the correlations (96) can be written as:

$$\tilde{G}\tilde{B}\bar{C} + \bar{C}\tilde{G}\tilde{B} = -I \tag{105}$$

where $\tilde{G}(x,y) = (1+\epsilon g[\phi;x])\delta(x-y)$. We look for perturbative solutions of this equation:

$$\bar{C} = \sum_{n=0}^{\infty}\epsilon^n\bar{C}_n. \tag{106}$$

After substituting the last expression into equation (105), we obtain order by order in ϵ the following hierarchy of equations:

$$\begin{aligned}
&\tilde{B}\bar{C}_0 + \bar{C}_0\tilde{B} = -I \\
&\tilde{B}\bar{C}_n + \bar{C}_n\tilde{B} = -G\tilde{B}\bar{C}_{n-1} - \bar{C}_{n-1}\tilde{B}G \quad n>0
\end{aligned} \tag{107}$$

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where $\tilde{G} = I + \epsilon G$ and $G(x, y) = g[\phi\,; x]\delta(x - y)$. The solutions are:

$$\begin{aligned} \bar{C}_0 &= -\frac{1}{2}\tilde{B}^{-1} \\ \bar{C}_n &= \int_0^\infty \mathrm{d}\alpha\, \mathrm{e}^{\alpha\tilde{B}} \left(G\tilde{B}\bar{C}_{n-1} + \bar{C}_{n-1}\tilde{B}G \right) \mathrm{e}^{\alpha\tilde{B}} \quad n > 0 \end{aligned} \tag{108}$$

and, in particular,

$$\bar{C}_1 = -\int_0^\infty \mathrm{d}\alpha\, \mathrm{e}^{\alpha\tilde{B}} G\, \mathrm{e}^{\alpha\tilde{B}} = QAQ^{\mathrm{T}} \tag{109}$$

where Q is the matrix that diagonalizes $\tilde{B}$: $\tilde{B} = QDQ^{\mathrm{T}}$; that is, $Q_{ij} = v_i(\lambda_j)$ where $v(\lambda)$ is the eigenfunction of $\tilde{B}$ with eigenvalue λ (all in a formal discrete notation) and

$$A_{i,j} = \frac{(Q^{\mathrm{T}}GQ)_{ij}}{\lambda_i + \lambda_j}. \tag{110}$$

Observe that $\tilde{B}$ is by construction a local functional. However, its eigenfunctions (that depend on the boundary conditions and the form of V_0) may be nonlocal. Therefore, the first correction to the correlations could be already quite singular. We can obtain more corrections $\bar{C}_n$ in the same spirit and we could study some general properties of $\bar{C}$ depending on the G and V_0. However, this is beyond the scope of this paper. We just wanted to show the possibility to introduce a perturbative scheme and to show the nontrivial changes that may appear in the behavior of the two-body correlations.

6.2. DD case

We substitute H from equation (16) into (92) and we obtain:

$$\int_\Lambda \mathrm{d}z\, [K(x, z)C_2(z, y) + K(y, z)C_2(z, x)] = -\sum_{i,j} \frac{\partial}{\partial x_i}\frac{\partial}{\partial y_j} [\chi_{ij}[\phi^*\,; x]\delta(x - y)] \tag{111}$$

where

$$K(x, y) = \frac{\delta}{\delta\phi(y)} \left(-\nabla \cdot G[\phi; x]\right)|_{\phi=\phi^*} \tag{112}$$

with ϕ^* the solution of $\nabla \cdot G[\phi^*\,; x] = 0$.

Many models are designed from a dynamic acting on the system's bulk and boundary conditions that drives the system to an equilibrium state in the DD case. Afterward, just by changing the boundary conditions, one manages to introduce to the system flows of energy, mass, etc so that the system is driven into a nonequilibrium stationary state. Other nonequilibrium stationary states are just due to a bulk dynamical mechanism that directly introduces some current into the system and/or breaks some symmetry. Moreover, DD permits models with a strictly conserved quantity, the average density, which introduces a kind of long-range interaction that affects the system correlations. Let us comment on these particular scenarios for the DD correlations.

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- Nonequilibrium stationary states driven by boundary conditions: let us assume first that the stationary state of our system is the equilibrium one with a given $V_0[\phi]$ for an appropriate set of boundary conditions. The bulk dynamics are defined by (G, χ) with

$$G_i[\phi; x] = -\frac{1}{2}\sum_j \chi_{ij}[\phi; x]\partial_j \frac{\delta V_0[\phi]}{\delta\phi(x)}. \tag{113}$$

We know that the corresponding two-body correlations are:

$$C_2^{\rm eq}(x, y) = V_2^{-1}(x, y; \phi^*_{\rm eq}), \quad V_2(x, y; \phi) = \frac{\delta^2 V_0[\phi]}{\delta\phi(x)\delta\phi(y)} \tag{114}$$

with $\phi^*_{\rm eq}$ the solution of $G[\phi^*_{\rm eq}; x] = 0$ (the current is equal to zero). If we change the boundary conditions, the system develops nonzero currents and, therefore, we have a nonequilibrium stationary state. We assume that the stationary state ϕ^* is given now by the solution of the equation $G[\phi^*; x] = J$ where J is a constant vector that is fixed by the boundary conditions. In this context, it is convenient to decompose the two-body correlation function into two terms:

$$C_2(x, y) = C_2^{\rm leq}(x, y) + C_{\rm D}(x, y), \quad C_2^{\rm leq}(x, y) = V_2^{-1}(x, y; \phi^*). \tag{115}$$

The first term is the *local equilibrium correlation*, which is the equilibrium correlation evaluated with the local values of the field ϕ^* as if the system were at equilibrium at x with $\phi_{\rm eq} = \phi^*(x)$. On the other hand, we see that $C_{\rm D} = 0$ when $J = 0$ by construction. That is, $C_{\rm D}(x, y)$ describes in some sense the far-from-equilibrium part of the correlations. When we substitute equations (115) into (111) we obtain the closed equation for $C_{\rm D}$:

$$\begin{aligned}
&\sum_i \frac{\partial}{\partial x_i}\left[\alpha_i[\phi^*; x]C_{\rm D}(x, y) + \frac{1}{2}\sum_j \chi_{ij}[\phi^*; x]\frac{\partial}{\partial x_j}\int_\Lambda {\rm d}z\, C_2^{\rm leq,-1}(x, z)C_{\rm D}(z, y)\right] \\
&\sum_i \frac{\partial}{\partial y_i}\left[\alpha_i[\phi^*; y]C_{\rm D}(x, y) + \frac{1}{2}\sum_j \chi_{ij}[\phi^*; y]\frac{\partial}{\partial x_j}\int_\Lambda {\rm d}z\, C_2^{\rm leq,-1}(y, z)C_{\rm D}(z, x)\right] \\
&\qquad = -\sum_i \frac{\partial}{\partial x_i}\left[\alpha_i[\phi^*; x]C_2^{\rm leq}(x, y)\right] - \sum_i \frac{\partial}{\partial y_i}\left[\alpha_i[\phi^*; y]C_2^{\rm leq}(x, y)\right]
\end{aligned} \tag{116}$$

where α is a d-dimensional vector

$$\alpha[\phi; x] = \chi'[\phi; x]\chi^{-1}[\phi; x]J \tag{117}$$

and we have considered that $\chi_{ij}[\phi\,; x]$ is a function that depends only on $\phi(x)$; that is, $\chi_{ij}[\phi\,; x] = \chi_{ij}(\phi(x))$. Therefore, $\chi'_{ij}[\phi\,; x] = \partial\chi_{ij}(u)/\partial u|_{u=\phi(x)}$.

The solution of this equation is very complex and it depends on the particular system and boundary conditions used. Let us explicitly work out a well-known particular case: the pure *diffusive system*, by taking:

$$V_0[\phi] = \int_\Lambda {\rm d}x\, [v(\phi(x)) - 2E \cdot x\phi(x)] \tag{118}$$

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where E is an external constant vector. With this choice we obtain:

$$G_i[\phi;x] = -\sum_j \left[D_{ij}[\phi;x]\partial_j\phi(x) - \chi_{ij}[\phi;x]E_j\right] \tag{119}$$

where

$$D[\phi;x] = \frac{1}{2}v''(\phi(x))\chi[\phi;x] \tag{120}$$

that is, the so-called *Einstein relation*. We observe that in equilibrium (with the appropriate boundary conditions) $\phi^*_{\rm eq}(x)$ is the solution of the *barometric equation*:

$$\nabla\phi^*_{\rm eq}(x) = -\frac{2}{Vv'(\phi^*_{\rm eq}(x))}E. \tag{121}$$

Moreover,

$$C_2^{\rm eq}(x,y) = \frac{1}{v''(\phi^*_{\rm eq}(x))}\delta(x-y). \tag{122}$$

In a nonequilibrium setup we obtain that the stationary state is a solution of the equation:

$$-\sum_j \left[D_{ij}[\phi^*;x]\partial_j\phi^*(x) - \chi_{ij}[\phi^*;x]E_j\right] = J_i \tag{123}$$

and the equation for $C_{\rm D}$ is, in this case:

$$\begin{aligned}\sum_{ij}\Bigg[\frac{\partial}{\partial x_i}\left[\frac{\partial(D_{ij}[\phi^*;x]C_{\rm D}(x,y))}{\partial x_j} - \chi'_{ij}[\phi^*;x]C_{\rm D}(x,y)\right]\\ + \frac{\partial}{\partial y_i}\left[\frac{\partial(D_{ij}[\phi^*;y]C_{\rm D}(x,y))}{\partial y_j} - \chi'_{ij}[\phi^*;y]C_{\rm D}(x,y)\right]\Bigg]\\ = \frac{1}{2}\left(\nabla\cdot\bar{\alpha}[\phi^*;x]\right)\delta(x-y)\end{aligned} \tag{124}$$

where

$$\bar{\alpha}[\phi;x] = \chi'[\phi;x]D^{-1}[\phi;x]J. \tag{125}$$

In particular, let us restrict to one dimension, $D = \text{cte}$, $E = 0$ and $\chi[\phi\,;x]$ a positive second-order polynomial of the form $\chi[\phi\,;x] = c_0 + c_1\phi(x) + c_2\phi(x)^2$. We find that $J = -D\,{\rm d}\phi^*(x)/{\rm d}x$. This implies a stationary state: $\phi^*(x) = \phi^*(0) - Jx/D$, $J = D(\phi^*(L) - \phi^*(0))/L$, where we have fixed the values of ϕ at the boundaries of the segment $[0, L]$. Then, the correlation function is

$$C_2(x,y) = \frac{\chi[\phi^*;x]}{2D}\delta(x-y) + C_{\rm D}(x,y) \tag{126}$$

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where the equation for $C_{\rm D}$ is reduced to:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mathrm{d}^2}{\mathrm{d}y^2}\right]C_{\rm D}(x,y)=-2\frac{J^2}{D^3}c_2\delta(x-y). \tag{127}$$

We can obtain an explicit solution for it (see, for instance, [19]):

$$C_{\rm D}(x,y)=-\frac{J^2}{D^3}c_2\Delta^{-1}(x,y) \tag{128}$$

with

$$\Delta^{-1}(x,y)=-\frac{1}{L}\left[(L-x)y\theta(x-y)+x(L-y)\theta(y-x)\right] \tag{129}$$

where $\theta(x)$ is the Heaviside function. Observe the long-range behavior of $C_{\rm D}$ and that its sign depends on the sign of c_2.

From this result we can obtain the fluctuations of the averaged field $\rho[\phi]=\frac{1}{L}\int_0^L \mathrm{d}x\,\phi(x)$:

$$\Sigma\equiv\Omega\langle(\rho[\phi]-\rho^*)^2\rangle_{st}=\frac{1}{L^2}\int_0^L \mathrm{d}x\int_0^L \mathrm{d}y\,C_2(x,y)\equiv\Sigma_{\rm leq}+\Sigma_{\rm D} \tag{130}$$

where

$$\begin{aligned}\Sigma_{\rm leq}&=\frac{1}{2DL}\left[c_0+c_1\rho^*+\frac{c_2}{3}\left(\phi^*(0)^2+\phi^*(0)\,\phi^*(1)+\phi^*(1)^2\right)\right]\\ \Sigma_{\rm D}&=\frac{c_2}{12DL}(\phi^*(0)-\phi^*(L))^2\end{aligned} \tag{131}$$

with $\rho^*=\rho[\phi^*]$. We see that the deviation from the local equilibrium is proportional to the square of the external gradient. This result has been derived in the boundary-driven symmetric simple exclusion process (SSEP) and in the KMP [19, 20, 26].

- Bulk nonequilibrium: let us focus on a very simple nonequilibrium model at the bulk level that develops highly nontrivial correlations. Let

$$G[\phi;x]=-D\nabla\phi \tag{132}$$

where we assume that D and χ are constant arbitrary d-dimensional matrices. One can easily check that this system is time-reversible if D is proportional to χ. Let us assume periodic boundary conditions such that $\phi^*(x)=\mathrm{cte}$ is the stationary state. Therefore, the currents on the system are zero: $G[\phi^*;x]=0$. The equation for C_2 is in this case given by:

$$\sum_{ij}D_{ij}\frac{\partial^2\bar{C}_2(x-y)}{\partial x_i\partial x_j}=\frac{1}{2}\sum_{ij}\chi_{ij}\frac{\partial^2\delta(x-y)}{\partial x_i\partial x_j} \tag{133}$$

where we have assumed that the correlations are translationally invariant: $C_2(x,y)=\bar{C}_2(x-y)$. The solution of equation (133) is given by:

$$\bar{C}_2(u)=\int \mathrm{d}k\,\mathrm{e}^{\mathrm{i}ku}\hat{C}_2(k),\quad \hat{C}_2(k)=\frac{k\cdot\chi k}{k\cdot Dk} \tag{134}$$

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We see that $\hat{C}_2$ is nonanalytic at $k = 0$ when D is not proportional to χ (this also implies D and/or χ to be anisotropic) and $\bar{C}_2(u)$ has a power-law decay behavior [25]. Let us remark on the fact that these very simple conservative dynamics with no macroscopic current have long-range correlations just by breaking the proportionality between D and χ. We can infer that equilibrium is reached by fine-tuning of the system's parameters and that the normal behavior is the nonequilibrium one.

- Strictly conserved models: DD models permits the average density

$$\frac{1}{|\Lambda|}\int_\Lambda \mathrm{d}x\, \phi(x,t) = \bar{\phi} \quad \forall\ t \tag{135}$$

to be strictly conserved under suitable boundary conditions (for instance, periodic). In this case, the stationary probability distribution can be written

$$P_{st}[\phi] \simeq \exp\left[-\Omega V_0[\phi]\right] \delta\left(\int_\Lambda \mathrm{d}x\, \phi(x) - |\Lambda|\bar{\phi}\right) \quad \Omega \to \infty \tag{136}$$

where $V_0[\phi]$ is the solution of the Hamilton–Jacobi equation:

$$H\left[\phi, \frac{\delta V_0[\phi]}{\delta \phi}\right] = 0 \tag{137}$$

with H given by equation (16). This slightly changes the initial assumption we used from equations (72) and (82) to derive the expressions for the correlations, and we need to reformulate them. The generating functional (85) can be written

$$Z[b] \propto \int D\phi \int \mathrm{d}s\, \exp\left[-\Omega \mathcal{F}[\phi, b, s]\right] \quad \Omega \to \infty \tag{138}$$

where

$$\mathcal{F}[\phi, b, s] = V_0[\phi] - \int_\Lambda \mathrm{d}x\, b(x)\phi(x) + s\left(\int_\Lambda \mathrm{d}x\, \phi(x) - |\Lambda|\bar{\phi}\right). \tag{139}$$

The two-body correlations are given by

$$C_2(x,y) = \lim_{\Omega\to\infty} \frac{\delta^2 I[b]}{\delta b(x)\delta b(y)}|_{b=0} \tag{140}$$

with

$$I[b] = \frac{1}{\Omega}\log Z[b] = -\mathcal{F}[\phi^*[b], b, s^*[b]] \tag{141}$$

and $(\phi^*[b], s^*[b])$ are the values that minimize $\mathcal{F}$:

$$\begin{aligned} &\frac{\delta V_0[\phi]}{\delta \phi(x)}|_{\phi=\phi^*[b]} = b(x) - s^*[b] \equiv \bar{b}(x) \\ &\int_\Lambda \mathrm{d}x\, \phi^*(x;b) = |\Lambda|\bar{\phi} \quad \forall\ b's. \end{aligned} \tag{142}$$

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We observe that $s^*[0] = 0$ and we can obtain $\phi^*[b]$ and $s^*[b]$ from equation (142) using a perturbative scheme around $\bar{b} = 0$:

$$\phi^*(x;b) = \phi^*(x) + \int_\Lambda \mathrm{d}y\, C_2^{\mathrm{NC}}(x,y)\bar{b}(y) + O(\bar{b}^2)$$
$$s^*[b] = \frac{\int_\Lambda \mathrm{d}x \int_\Lambda \mathrm{d}y\, C_2^{\mathrm{NC}}(x,y)\bar{b}(y)}{\int_\Lambda \mathrm{d}x \int_\Lambda \mathrm{d}y\, C_2^{\mathrm{NC}}(x,y)} + O(\bar{b}^2) \tag{143}$$

where

$$C_2^{\mathrm{NC}}(x,y) = V_2^{-1}(x,y) \tag{144}$$

and V_2 is given by equation (75). That is, C_2^{NC} is the two-body correlation function corresponding to a system with the same dynamics and boundaries as the original system but without the density conservation condition (observe that V_0 is computed using the Hamilton–Jacobi equation (137) where $\bar{\phi}$ is fixed when the stationary state is chosen). Finally, we obtain C_2 by performing the expansion of $I[b]$ (141) up to the second order in $\bar{b}$ of their arguments:

$$C_2(x,y) = C_2^{\mathrm{NC}}(x,y) - \frac{\int_\Lambda \mathrm{d}\bar{y}\, C_2^{\mathrm{NC}}(x,\bar{y}) \int_\Lambda \mathrm{d}\bar{x}\, C_2^{\mathrm{NC}}(\bar{x},y)}{\int_\Lambda \mathrm{d}\bar{x} \int_\Lambda \mathrm{d}\bar{y}\, C_2^{\mathrm{NC}}(\bar{x},\bar{y})}. \tag{145}$$

We see that $\int_\Lambda \mathrm{d}x\, C_2(x,y) = \int_\Lambda \mathrm{d}y\, C_2(x,y) = 0$ as expected. Observe also that the difference between C_2 and C_2^{NC} is of order $|\Lambda|^{-1}$ and, therefore, both correlations coincide in the thermodynamic limit $|\Lambda| \to \infty$. At the practical level, the condition of density conservation does not change the fact that first we should obtain C_2^{NC} from equation (111) as in the other cases and the system's physics are completely characterized by it.

6.3. Initial approach to define nonequilibrium dynamical ensembles

We know from the equilibrium ensemble theory that there are several probability densities defined in the configurational space that give rise to the same macroscopic description in the thermodynamic limit [27]. For instance, we are aware of the microcanonical, canonical, and grand canonical ensembles. The same Hamiltonian characterizes all the ensembles at the microscopic level, and their differences are in the constraints they have as the conservation of energy, of particles, etc. This equivalence can also be transported to dynamic equations. For example, we can build several stochastic dynamics to drive the system to the same equilibrium state. At the mesoscopic level, we have already seen that RD and DD systems at equilibrium have the same stationary distribution defined by the quasipotential $V_0[\phi]$ (except for a DD with strict conservation where the conservation of the field appears explicitly and it affects the system correlations in a controlled manner). In any case, all of them describe the same macroscopic state at the thermodynamic limit: their deterministic values and their correlations are equal.

The equivalence of ensembles in nonequilibrium systems has been studied from several different points of view. Let us comment, for example, on the comparison of turbulent Navier–Stokes hydrodynamic equations with different forcing and dissipative

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mechanisms with equal averages for any reasonable observable [28], or the construction of equivalent *biased* dynamics at the level of path's probabilities for Markov processes when a constraint is included on a time-averaged observable that gives rise to the same large deviation distribution [29].

Here, we question the possibility of obtaining a couple of RD and DD dynamics that drive a system to the same nonequilibrium stationary state. We assume that there are two levels of equivalence: (i) the strong equivalence where the quasipotential V_0 is the same in RD and DD models except for a conservation constraint if necessary (see equation (136)), and (ii) the weak equivalence where we look for RD and DD models that have the same macroscopic stationary state and two-body correlations. Showing the strong equivalence for a couple of dynamics is a nontrivial task because of the nonlocal structure of V_0. Therefore, it depends on the boundary conditions and the details of the dynamics. For this reason, it is more convenient to first explore the weak equivalence by looking for the conditions under which the RD and DD systems have equal two-body correlations (observe that if we consider a DD with strict conservation of density, we want to compare the RD correlation function with the DD's correlation $C_2^{\rm NC}$).

The two-body correlation is the solution of equation (92), each one with their own Hamiltonian. This implies equations (93) and (111) for the RD and DD systems, respectively. We do not know how to solve such equations in general except in the RD case when the B kernel (95) is symmetric. That restricts a lot of the types of nonequilibrium models we can study. Nevertheless, it gives us some interesting insights into the conditions for the existence of a weak equivalence.

Let us assume RD dynamics defined by $F[\phi\,;x]$ and $h[\phi\,;x]$ functionals with the property:

$$B(x,y) \equiv \frac{h[\phi_1^*;y]}{h[\phi_1^*;x]}\frac{\delta F[\phi;x]}{\delta\phi(y)}|_{\phi=\phi_1^*} = B(y,x) \tag{146}$$

where ϕ_1^* is the solution of $F[\phi_1^*;x]=0$. We showed above that in this case the two-body correlations are given by:

$$C_2(x,y) = -\frac{1}{2}h[\phi_1^*;x]h[\phi_1^*;y]B^{-1}(x,y). \tag{147}$$

We impose that this correlation should also be a solution of equation (111) for the two-body correlations in the DD case (defined by $G[\phi\,;x]$ and $\chi_{ij}[\phi\,;x]$ functionals). Obviously, the boundary conditions for C_2 are equal in both cases. In this way we obtain the relation:

$$h[\phi_1^*;y]\int_\Lambda {\rm d}z\, K(x,z)h[\phi_1^*;z]B^{-1}(z,y) = \sum_{ij}\frac{\partial}{\partial x_i}\frac{\partial}{\partial y_j}\left[\chi_{ij}[\phi_2^*;x]\delta(x-y)\right] \tag{148}$$

where

$$K(x,y) = \frac{\delta}{\delta\phi(y)}\left(-\nabla\cdot G[\phi;x]\right)|_{\phi=\phi_2^*} \tag{149}$$

with ϕ_2^* solution of $\nabla\cdot G[\phi_2^*;x]=0$. After some trivial algebra, we find that the RD with (F,h) and DD with (G,χ) have the same C_2 correlation provided that the following

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relationship is fulfilled:

$$\frac{\delta G_i[\phi;x]}{\delta\phi(y)}|_{\phi=\phi_2^*}=\sum_j\chi_{ij}[\phi_2^*;x]\frac{\partial}{\partial x_j}\left[\frac{1}{h[\phi_1^*;x]^2}\frac{\delta F[\phi;x]}{\delta\phi(y)}|_{\phi=\phi_1^*}\right]. \tag{150}$$

One can also check that

$$G_i[\phi;x]=\sum_j\chi_{ij}[\phi;x]\frac{\partial}{\partial x_j}\left[\frac{F[\phi;x]}{h[\phi;x]^2}\right] \tag{151}$$

fulfills relation (150). Observe that in this case the deterministic solutions for the RD and DD models coincide: $\phi_1^*=\phi_2^*=\phi^*$. In conclusion, we have shown the following property:

- All RD models with a symmetric B-kernel (146) have an associated DD model given by (151) such that both have the same macroscopic state and two-body correlations and therefore they are, at least, weak-equivalent.

We can apply this property to the equilibrium case where F is of the form:

$$F[\phi;x]=-\frac{1}{2}h[\phi;x]^2\frac{\delta V[\phi]}{\delta\phi(x)} \tag{152}$$

for any arbitrary h and V functionals. The B-kernel (151) is in this case always symmetric and the weak equivalent conservative dynamics are the expected:

$$G_i[\phi;x]=-\frac{1}{2}\sum_j\chi_{ij}[\phi;x]\frac{\partial}{\partial x_j}\left[\frac{\delta V[\phi]}{\delta\phi(x)}\right] \tag{153}$$

(see equation (70)). We know that both dynamics have the same quasipotential: $V_0[\phi]=V[\phi]$. That is, they are also strong-equivalent.

Let us see what happens for a simple RD system with a nonequilibrium stationary state. We assume that RD is defined by (F,h) where

$$F[\phi;x]=-\frac{1}{2}g[\phi;x]^2\frac{\delta V[\phi]}{\delta\phi(x)} \tag{154}$$

with $V[\phi]$, $g[\phi\,;x]$ and $h[\phi\,;x]$ are given functionals. We know that whenever $g[\phi\,;x]\neq h[\phi\,;x]$ the system is in a nonequilibrium stationary state and the quasipotential $V_0[\phi]\neq V[\phi]$. The B-kernel (146) is in this case

$$B(x,y)=-\frac{1}{2}\frac{h[\phi^*;y]}{h[\phi^*;x]}g[\phi^*;x]^2\frac{\delta^2V[\phi]}{\delta\phi(x)\delta\phi(y)}|_{\phi=\phi^*} \tag{155}$$

and it is symmetric when the deterministic solution is spatially homogeneous $\phi^*(x)=\phi^*=\text{cte}$. In this case we apply the result (151) and the DD dynamics with the same two-body correlations as the RD are:

$$G_i[\phi;x]=-\frac{1}{2}\sum_j\chi_{ij}[\phi;x]\frac{\partial}{\partial x_j}\left[\frac{g[\phi;x]^2}{h[\phi;x]^2}\frac{\delta V[\phi]}{\delta\phi(x)}\right] \tag{156}$$

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for any given χ_{ij}. It is an open problem to see if there is a strong equivalence in this case. We have just shown with this example that there exists a weak equivalence between a family of RD and DD systems. It seems interesting to explore the possibility of finding such an equivalence in more complex dynamics.

7. Conclusions

We have attempted to show nonequilibrium systems' general properties in stationary states, assuming that continuum Langevin equations describe them. We have studied the stationary measure at the small noise limit through the quasipotential. This object is a natural extension of the free energy functional for systems in equilibrium. A quasipotential typically has a nonlocal structure, a strong dependence on the boundary conditions, and the dynamics' details. Finally, it may contain some nondifferential behavior. These properties make it very difficult to devise an *a priori* way of building them from first principles as it occurs for the equilibrium. That prevents us from using the quasipotentials as a starting point to develop hypothetical nonequilibrium thermodynamics. We show how the most probable path to creating a fluctuation from the stationary state is, for nonequilibrium systems, different from the most probable path to relax from it. When both coincide, the system is called *macroscopically time-reversible*. This property is not enough to discriminate nonequilibrium stationary states from the equilibrium. To do that, one should introduce the *adjoint dynamics* as the Langevin equation for the time-reversed process. In this way, equilibrium is defined as the process in which the Langevin dynamics coincide with their adjoint. The stationary two-body correlations characterize the quasipotential near the stationary state. We have explicitly built the equations to derive them, studying several properties, examples, and even perturbation schemes to show their richness and nontrivial behavior.

This work aims to show a systematic way to study nonequilibrium systems from a theoretical point of view. It gives us the possibility to study different nonequilibrium models under the same scheme and compare them to look for their common regularities. Moreover, the advantage of this common theoretical ground is that any exact resolution, approximation, perturbation scheme, or assumption can be checked in many different scientific contexts from numerical models or real experiments.

Finally, it is also observed that small changes in the overall functionals may imply large differences in the kind of results we derive from the theory. Therefore, one of the main questions to be solved is to determine the influence of the underlying microscopic details in the mesoscopic description. We know that in some important cases of boundary-driven nonequilibrium systems (for example, fluctuating hydrodynamics [30]), the mesoscopic theory contains most of the necessary elements to correctly describe many observed phenomena. Nevertheless, we would like to have an *a priori* predictive way to connect the microscopic and mesoscopic descriptions safely.

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Appendix A. From Langevin to Fokker Planck equations through a family of discretization schemes

A.1. RD case

Let us assume that the Langevin equation (5) is the continuous limit of its time-discrete version:

$$\phi(x,s+1)=\phi(x,s)+\epsilon\left[F[\phi;x,s,v]+h[\phi;x,s,v]\xi(x,s)\right] \tag{157}$$

where we also assume:

$$\begin{aligned} F[\phi;x,s,v] &= F[v\phi(x,s)+(1-v)\phi(x,s+1);x] \\ h[\phi;x,s,v] &= h(v\phi(x,s)+(1-v)\phi(x,s+1)) \end{aligned} \tag{158}$$

with $v\in[0,1]$, $x\in\Lambda\subset IR^d$, $s\in Z$ and $F[\phi\,;x]$ is a functional on $\phi(y)$'s with y pertaining to a finite open region around x while $h(\lambda)$ is a function. The random field ξ is Gaussian white noise characterized by:

$$\langle\xi(x,s)\rangle=0,\quad \langle\xi(x,s)\xi(x',s')\rangle=\frac{1}{\epsilon\Omega}\delta(x,x')\delta_{s,s'}. \tag{159}$$

Observe that for any value $v\in[0,1]$ the limit $\epsilon\to 0$ of this discrete equation gives rise to the continuous Langevin equation (5).

We can expand the Langevin equation (157) in powers of ϵ:

$$\begin{aligned} \phi\left(x,s+1\right) &= \phi\left(x,s\right)+\epsilon h\left(\phi\left(x,s\right)\right)\xi\left(x,s\right)+\epsilon F[\phi;x,s] \\ &\quad +\left(1-v\right)\epsilon^2 h\left(\phi\left(x,s\right)\right)h'\left(\phi\left(x,s\right)\right)\xi(x,s)^2+O\left(\epsilon^{3/2}\right) \end{aligned} \tag{160}$$

where we have assumed that ξ is of order $\epsilon^{-1/2}$.

The probability of finding a given configuration ϕ at time s is defined by

$$P[\phi;s+1]=\left\langle\prod_{x\in\Lambda}\delta(\phi(x)-\phi(x,s+1))\right\rangle_\xi \tag{161}$$

where $\phi(x,s)$ is the solution of the Langevin equation for a given random noise realization and $\langle\cdot\rangle_\xi$ is the average over all noise realizations with their corresponding Gaussian weight. We can substitute the ϵ expanded Langevin equation into equation (161) and after some algebraic manipulation we obtain

$$\begin{aligned} P[\phi;s+1]=\int\prod_{x\in\Lambda}\left[\mathrm{d}\bar{\phi}\left(x\right)\right]P[\bar{\phi};s]\Bigg\langle\prod_{x\in\Lambda}\delta\left(\phi\left(x\right)-\bar{\phi}\left(x\right)-\epsilon h\left(\bar{\phi}\left(x\right)\right)\xi\left(x,s\right)-\epsilon F[\bar{\phi};x]\right. \\ \left.-\left(1-v\right)\epsilon^2 h\left(\bar{\phi}\left(x\right)\right)h'\left(\bar{\phi}\left(x\right)\right)\xi(x,s)^2+O\left(\epsilon^{3/2}\right)\right)\Bigg\rangle_\xi. \end{aligned} \tag{162}$$

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We have used the fact that $\phi(x,s)$ only depends on ξ's of previous times, $s' < s$, and therefore, we can break the averages over ξ's. We expand the last expression with respect to ϵ by using the perturbative formula:

$$\prod_n \delta(a(n)+b(n)\eta+c(n)\eta^2) = \left(\prod_n \delta(a(n))\right) + \eta \sum_m \left(\prod_{n\neq m} \delta(a(n))\right) \delta'(a(m))b(m) + \frac{1}{2}\eta^2 \times \sum_m \left[\left(\prod_{n\neq m} \delta(a(n))\right)\left[\delta''(a(m))b(m)^2 + 2\delta'(a(m))c(m)\right] + \sum_{m'\neq m} \left(\prod_{n\neq m,m'} \delta(a(n))\right) \delta'(a(m))\delta'(a(m'))b(m)b(m')\right] + O(\eta^3) \tag{163}$$

that we obtain by performing the first two derivatives with respect to η on the right-hand side of equation (163) and expanding the remaining expression up to the second order in η. In our case we identify $\eta = \epsilon^{1/2}$.

Finally, we can calculate the averages over ξ's and we obtain (in the limit $\epsilon \to 0$) the Fokker–Planck equation:

$$\partial_t P[\phi;t] = \int_\Lambda \mathrm{d}x \, \frac{\delta}{\delta\phi(x)} \left[-(F[\phi;x] + \frac{(1-v)}{\Omega} h(\phi(x))h'(\phi(x)))P[\phi;t] + \frac{1}{2\Omega}\frac{\delta}{\delta\phi(x)}\left(h(\phi(x))^2 P[\phi;t]\right)\right]. \tag{164}$$

One can show that the observables (averages) computed with this Lagrangian do not depend on the v used [31]. For $v = 1$ (Ito's discretization) we obtain the Fokker–Planck equation that is used in this paper:

$$\partial_t P[\phi;t] = \int_\Lambda \mathrm{d}x \, \frac{\delta}{\delta\phi(x,t)} \left[-F[\phi;x,t]P[\phi;t] + \frac{1}{2\Omega}\frac{\delta}{\delta\phi(x,t)}\left(h[\phi;x,t]^2 P[\phi;t]\right)\right]. \tag{165}$$

A.2. DD case

In this case it is necessary to define space and time discretizations. The field at lattice site $n \in Z^d$ at discrete time $s \in Z$, $\phi(n,s)$ is a solution of the discrete Langevin equation:

$$\phi(n,s+1) = \phi(n,s) - \frac{\epsilon}{2a}\sum_{\alpha=1}^{d} \left[j_\alpha(\phi;n+i_\alpha,s) - j_\alpha(\phi;n-i_\alpha,s)\right] \tag{166}$$

where i_α is the unit vector in the direction α and

$$j_\alpha(\phi;n,s) = G_\alpha[\phi;n,s] + \sum_{\beta=1}^{d} \sigma_{\alpha\beta}[\phi;n,s]\psi_\beta(n,s) \tag{167}$$

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$$\langle \psi_\alpha(n,s)\psi_\beta(n',s')\rangle = \frac{1}{\tilde{\Omega}\epsilon a^d}\delta_{\alpha,\beta}\delta_{n,n'}\delta_{s,s'} \tag{168}$$

where a and ϵ are the lattice node separations in space and time, respectively. For simplicity we are considering just Ito's scheme.

The probability of finding a given configuration ϕ at time s is defined by

$$P[\phi; s+1] = \left\langle \prod_{n\in\Lambda} \delta(\phi(n) - \phi(n, s+1)) \right\rangle_\psi \tag{169}$$

where $\phi(n,s)$ is the solution of the Langevin equation for a given random noise realization; that is, it depends on ψ and $\langle\cdot\rangle_\psi$ is the average over all noise realizations with their corresponding Gaussian weight. We can insert the right-hand side of the Langevin equation and we introduce an auxiliary field $\bar{\phi}$:

$$P[\phi; s+1] = \left\langle \int \prod_{n\in\Lambda} \left[\mathrm{d}^-\phi(n)\delta(\bar{\phi}(n) - \phi(n,s))\right] \times \prod_{n\in\Lambda} \delta\left(\phi(n) - \bar{\phi}(n) + \frac{\epsilon}{2a}\sum_{\alpha=1}^{d}\left[j_\alpha(\bar{\phi}; n+i_\alpha) - j_\alpha(\bar{\phi}; n-i_\alpha)\right]\right)\right\rangle_\psi . \tag{170}$$

We use the fact that the noise ψ is time-uncorrelated and Ito's prescription. Moreover, $\phi(n,s)$ only depends on ψ's with times strictly smaller than s. Therefore, we can break the average over ψ and we obtain:

$$P[\phi; s+1] = \int \prod_{n\in\Lambda} \left[\mathrm{d}^-\phi(n)\right] P[\bar{\phi}; s] \times \left\langle \prod_{n\in\Lambda} \delta\left(\phi(n) - \bar{\phi}(n) + \frac{\epsilon}{2a}\sum_{\alpha=1}^{d}\left[j_\alpha(\bar{\phi}; n+i_\alpha) - j_\alpha(\bar{\phi}; n-i_\alpha)\right]\right)\right\rangle_\psi . \tag{171}$$

We expand the last expression for $\epsilon \leqslant 1$, taking into account that ψ is of order $\epsilon^{-1/2}$. We can use formula (163) with

$$\begin{aligned} a(n) &= \phi(n) - \bar{\phi}(n) \\ b(n) &= \frac{\epsilon^{1/2}}{2a}\sum_{\alpha=1}^{d}\sum_{\beta=1}^{d}\left[\sigma_{\alpha\beta}[\bar{\phi}; n+i_\alpha]\psi_\beta(n+i_\alpha, s) - \sigma_{\alpha\beta}[\bar{\phi}; n-i_\alpha]\psi_\beta(n-i_\alpha, s)\right] \\ c(n) &= \frac{1}{2a}\sum_{\alpha=1}^{d}\left[G_\alpha[\bar{\phi}; n+i_\alpha] - G_\alpha[\bar{\phi}; n-i_\alpha]\right] . \end{aligned} \tag{172}$$

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After substituting this expansion into equation (171) we can explicitly calculate the averages over ψ and after some algebra we obtain

$$\begin{aligned} P[\phi;s+1] = P[\phi;s] + \epsilon \sum_{m\in\Lambda} \frac{\partial}{\partial\phi(m)} \Bigg[P[\phi;s] \frac{1}{2a} \sum_{\alpha=1}^{d} \left(G_\alpha[\phi;n+i_\alpha] - G_\alpha[\phi;n-i_\alpha] \right) \\ + \frac{1}{8\tilde{\Omega}a^{d+2}} \sum_{\alpha=1}^{d}\sum_{\beta=1}^{d} \Bigg(\frac{\partial}{\partial\phi(m+i_\alpha-i_\beta)} \left(P[\phi;s]\chi_{\alpha\beta}[\phi;m+i_\alpha] \right) \\ - \frac{\partial}{\partial\phi(m+i_\alpha+i_\beta)} \left(P[\phi;s]\chi_{\alpha\beta}[\phi;m+i_\alpha] \right) \\ - \frac{\partial}{\partial\phi(m-i_\alpha-i_\beta)} \left(P[\phi;s]\chi_{\alpha\beta}[\phi;m-i_\alpha] \right) \\ + \frac{\partial}{\partial\phi(m-i_\alpha+i_\beta)} \left(P[\phi;s]\chi_{\alpha\beta}[\phi;m-i_\alpha] \right) \Bigg) \Bigg] + O(\epsilon^2) \end{aligned} \tag{173}$$

where

$$\chi_{\alpha\beta}[\phi;n] = \sum_{\gamma=1}^{d} \sigma_{\alpha\gamma}[\phi;n]\sigma_{\beta\gamma}[\phi;n]. \tag{174}$$

This expression can be written in a more compact form using the definition:

$$\left(\partial_\alpha \frac{\partial}{\partial\phi(n)} \right) \equiv \frac{1}{2a} \left(\frac{\partial}{\partial\phi(n+i_\alpha)} - \frac{\partial}{\partial\phi(n-i_\alpha)} \right). \tag{175}$$

Therefore, we obtain

$$\begin{aligned} \frac{1}{\epsilon} \left[P[\phi;s+1] - P[\phi;s] \right] = \sum_{\alpha=1}^{d}\sum_{m\in\Lambda} \left(\partial_\alpha \frac{\partial}{\partial\phi(m)} \right) \left[-G_\alpha[\phi;m]P[\phi;s] \right. \\ \left. + \frac{1}{2\tilde{\Omega}a^d} \sum_{\beta=1}^{d} \left(\partial_\beta \frac{\partial}{\partial\phi(m)} \right) \left(\chi_{\alpha\beta}[\phi;m]P[\phi;s] \right) \right] + O(\epsilon). \end{aligned} \tag{176}$$

where we have used the properties:

$$\begin{aligned} \sum_{m\in\Lambda} \frac{\partial}{\partial\phi(m)} \left(\partial_\alpha G[\phi;m] \right) = -\sum_{m\in\Lambda} \left(\partial_\alpha \frac{\partial}{\partial\phi(m)} \right) G[\phi;m] \\ \left(\partial_\alpha \frac{\partial}{\partial\phi(m)} \right) \left(Q[\phi]F(\phi(m)) \right) = F(\phi(m))\partial_\alpha \left(\frac{\partial Q[\phi]}{\partial\phi(m)} \right) \end{aligned} \tag{177}$$

with $F(\lambda)$ being a function.

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In the limit $\epsilon \to 0$ and $a \to 0$, and defining $\tilde{\Omega} = a^d \Omega$, we recover the Fokker–Planck equation for diffusive systems:

$$\partial_t P[\phi;t] = \int_\Lambda \mathrm{d}x \sum_{\alpha=1}^{d} \left(\partial_\alpha \frac{\delta}{\delta\phi(x,t)}\right) \left[-G_\alpha[\phi;x,t]P[\phi;t] + \frac{1}{2\Omega}\sum_{\beta=1}^{d}\left(\partial_\beta \frac{\delta}{\delta\phi(x,t)}\right)\left(\chi_{\alpha,\beta}[\phi;x,t]P[\phi;t]\right)\right] \tag{178}$$

where

$$\chi_{\alpha,\beta}[\phi;x,t] = \sum_{\gamma=1}^{d} \sigma_{\alpha,\gamma}[\phi;x,t]\sigma_{\beta,\gamma}[\phi;x,t] \tag{179}$$

and

$$\left(\partial_\alpha \frac{\delta}{\delta\phi(x)}\right) = \lim_{a\to 0} \frac{1}{2a}\left(\frac{\partial}{\partial\phi(n+i_\alpha)} - \frac{\partial}{\partial\phi(n-i_\alpha)}\right) \tag{180}$$

where $x = na$. This operator has the useful property

$$\left(\partial_\alpha \frac{\delta}{\delta\phi(x,t)}\right) H[\phi;x,t] = \partial_\alpha\left(\frac{\delta}{\delta\phi(x,t)} H[\phi;x,t]\right) - \frac{\delta}{\delta\phi(x,t)}\left(\partial_\alpha H[\phi;x,t]\right). \tag{181}$$

Appendix B. Large deviations and Green–Kubo relations

Let us define the bulk average of an observable $a[\phi\,;x,t]$ for a given time t:

$$a[\phi;t] = \frac{1}{\Lambda}\int_\Lambda \mathrm{d}x\, a[\phi;x,t]. \tag{182}$$

Its time average over the time interval $[0,T]$ is then

$$a_T[\phi] = \frac{1}{T}\int_0^T \mathrm{d}t\, a[\phi;t]. \tag{183}$$

If the stochastic model is well behaved, we can apply the law of large numbers in the sense that

$$a^* \equiv \langle a[\phi;0]\rangle_{ss} = \lim_{T\to\infty} a_T[\phi]. \tag{184}$$

The probability to observe a certain value of $a_T[\phi] = a$ assuming that at time $t = 0$ the system is at the stationary state is given by:

$$P(a;T) = \int D\phi[0,T] P_{ss}[\phi(0)] P[\{\phi\}[0,T]]\delta(a - a_T[\phi]). \tag{185}$$

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The large deviation principle states that for large values of T this distribution should be very peaked around a^*. In fact, in such a limit it should be of the form:

$$P(a;T) \simeq \mathrm{e}^{-TR(a)} \quad T \to \infty \tag{186}$$

with

$$R(a^*) = 0 \qquad R'(a^*) = 0. \tag{187}$$

Therefore,

$$\lim_{T\to\infty} T\left\langle (a-a^*)^2 \right\rangle_P = R''(a^*)^{-1} \tag{188}$$

where $\langle\cdot\rangle_P$ means the average is done with the $P(a;T)$ distribution. We can now substitute $P(a,T)$ for its path definition and we obtain the Green–Kubo relation:

$$\frac{1}{2R''(a^*)} = \int_0^\infty \mathrm{d}\tau \, \langle (a[\phi;0]-a^*)(a[\phi;\tau]-a^*)\rangle \tag{189}$$

where now $\langle\cdot\rangle$ is the path average defined above.

We can apply this scheme to our RD and DD models and obtain (for a given $a[\phi\,;x,t]$) the function $R(a)$. As an example, let us study only an RD system with

$$\begin{aligned} a[\phi;x,t] &\to \phi(x,t) \\ a[\phi;t] &\to \rho[\phi;t] = \frac{1}{\Lambda}\int_\Lambda \mathrm{d}x\, \phi(x,t) \\ a_T[\phi] &\to \rho_T[\phi] = \frac{1}{T}\int_0^T \mathrm{d}t\, \rho[\phi;t] \end{aligned} \tag{190}$$

and $P[\{\phi\}[0,T]]$ is given by equation (9). The probability of observing a given average density over the space and a time interval T at the stationary state $\rho_T[\phi] = \rho$ is:

$$P[\rho;T] = \int D\phi[0,T] P_{ss}[\phi(0)] \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \frac{\mathrm{d}\lambda}{2\pi\mathrm{i}} \exp\left[-\Omega T R[\{\phi\}[0,T]]\right] \tag{191}$$

where

$$R[\{\phi\}[0,T],\lambda] = \frac{1}{2T}\int_0^T \mathrm{d}t \int_\Lambda \mathrm{d}x \left(\frac{\partial_t\phi(x,t) - F[\phi;x,t]}{h[\phi;x,t]}\right)^2 + \lambda\left(\rho - \rho_T[\phi]\right) \tag{192}$$

and we have used in equation (185) the representation of the Dirac delta by the integral on λ. We can explicitly compute $P[\rho\,;T]$ when $T\to\infty$ because the integrals are dominated by its minimum value over the fields and λ. That is,

$$P[\rho,T] \simeq \exp[-\Omega T R[\{\tilde{\phi}\}[0,T],\tilde{\lambda}]] \tag{193}$$

where $\tilde{\phi}$ and $\tilde{\lambda}$ are solutions of

$$\frac{\delta R}{\delta\phi(y,\tau)}|_{\phi=\tilde{\phi},\lambda=\tilde{\lambda}}=0, \qquad \frac{\partial R}{\partial\lambda}|_{\phi=\tilde{\phi},\lambda=\tilde{\lambda}}=0. \tag{194}$$

In general, these sets of equations have many different types of solutions (see, for instance, [32]), static and dynamic, that are local extremals of R. It is a daunting practical task to obtain solutions and check which one is the absolute minimum for R. Let us assume the simplest case in which the deterministic solution of the Langevin equation is constant in space: $\phi^*(x,t)=\rho^*=\text{cte}$. Obviously, when $\rho=\rho^*$ we expect that $\tilde{\phi}(x,t)=\rho^*$. For values of ρ near the stationary state solution ρ^* we can assume by continuity that $\tilde{\phi}(x,t)=\rho$ is a solution of the equations. This ansatz is the so-called *additivity principle* [33]. In this case

$$R[\{\tilde{\phi}\}[0,T],\tilde{\lambda}]=\Lambda\frac{F[\rho]^2}{2h[\rho]^2}\equiv R[\rho]. \tag{195}$$

Therefore,

$$R''[\rho^*]=\Lambda\frac{F'[\rho^*]^2}{h[\rho^*]} \tag{196}$$

and the Green–Kubo relation is

$$\frac{h[\rho^*]^2}{F'[\rho^*]^2}=2\Omega\int_{R^d}\mathrm{d}x\int_0^\infty\mathrm{d}\tau\,\langle(\phi(0,0)-\phi^*)(\phi(x,\tau)-\phi^*)\rangle \tag{197}$$

in the limit $\Lambda\to\infty$ and assuming spatial translation invariance.

We can similarly study different observables. In the DD case the time averaged mean current in some 1-d systems has been studied extensively [34]:

$$J_T[\phi]=\frac{1}{T\Lambda}\int_0^T\mathrm{d}t\int_\Lambda\mathrm{d}x\,j(x,t). \tag{198}$$

In one dimension, it is shown that the additivity principle is correct when we look for fluctuations of the current near the stationary value, but, in general, it fails for large current fluctuations where the solutions that minimize the functional R are much more complex than the uniform solution. For instance, this occurs when we use periodic boundary conditions where such solutions are soliton-like functions that move around the system at a constant speed. Moreover, it has been shown that in two dimensions, the KMP model [26] with a thermal gradient in one direction and periodic boundary conditions in the other presents a solution (*weak additivity principle*) that is not spatially uniform but is a better minimizer than the uniform solution even near the stationary value [35].

Appendix C. Method of characteristics to solve Hamilton–Jacobi equations

We reproduce page 233 in Gallavotti's book *Elements of Mechanics* [36]. Let $S(q,t)$ be a solution of the Hamilton–Jacobi equation

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$$H\left(\frac{\partial S(q,t)}{\partial q},q,t\right)+\frac{\partial S(q,t)}{\partial t}=0 \tag{199}$$

where $H=H(p,q,t)$ is a given function on its arguments. Let us assume the following differential equation:

$$\frac{\mathrm{d}q}{\mathrm{d}t}=\left.\frac{\partial H}{\partial p}\right|_{p=\frac{\partial S}{\partial q}} \tag{200}$$

with the initial condition $q(t_0)=q_0$. Then, we can show that if we take

$$p(t)=\left.\frac{\partial S}{\partial q}\right|_{q=q(t)} \tag{201}$$

with $q(t)$ the solution of equation (200), the functions $(q(t),p(t))$ are *solutions* of the Hamilton equations with Hamiltonian $H(p,q,t)$ and initial values $q(t_0)=q_0$ and $p(t_0)=\partial S/\partial q|_{q=q_0}$. That is, each solution of the Hamilton–Jacobi equation (199) corresponds to a Hamiltonian dynamic.

In order to show this assertion, we check that $p(t)$ so defined is a solution of the corresponding Hamilton equation $\mathrm{d}p/\mathrm{d}t=-\partial H/\partial q$:

$$\frac{\mathrm{d}p_i}{\mathrm{d}t}=\frac{\mathrm{d}}{\mathrm{d}t}\left(\left.\frac{\partial S}{\partial q_i}\right|_{q=q(t)}\right)=\sum_j\frac{\partial^2 S}{\partial q_i\partial q_j}\frac{\mathrm{d}q_j}{\mathrm{d}t}+\frac{\partial^2 S}{\partial t\partial q_i} \tag{202}$$

but deriving the Hamilton–Jacobi equation by $\partial/\partial q_i$ we find the relation:

$$\sum_j\frac{\partial^2 S}{\partial q_i\partial q_j}\frac{\mathrm{d}q_j}{\mathrm{d}t}+\left.\frac{\partial H(p,q,t)}{\partial q_i}\right|_{p=\frac{\partial S}{\partial q}}+\frac{\partial^2 S}{\partial t\partial q_i}=0 \tag{203}$$

that we can use in equation (202) to obtain the desired result:

$$\frac{\mathrm{d}p_i}{\mathrm{d}t}=-\frac{\partial H(p,q,t)}{\partial q_i},\qquad \frac{\mathrm{d}q_i}{\mathrm{d}t}=\frac{\partial H(p,q,t)}{\partial p_i} \tag{204}$$

with the above-mentioned initial conditions. In the case of a time-independent Hamiltonian, $S(q,t)=W(q)-\alpha t$, where α is a constant fixed at the initial time.

We can find $S(q,t)$ just by studying the time behavior of $S(q(t),t)$ with $q(t)$ the solution of the Hamilton equations:

$$\frac{\mathrm{d}S(q(t),t)}{\mathrm{d}t}=\sum_i\left.\frac{\partial S(q,t)}{\partial q_i}\right|_{q=q(t)}\frac{\mathrm{d}q_i}{\mathrm{d}t}+\left.\frac{\partial S(q,t)}{\partial t}\right|_{q=q(t)}. \tag{205}$$

We perform a time integration on it and obtain:

$$S(q(t),t)-S(q(t_0),t_0)=\int_{t_0}^{t}\mathrm{d}\tau\sum_i p_i(\tau)\frac{\mathrm{d}q_i(\tau)}{\mathrm{d}\tau}+\int_{t_0}^{t}\mathrm{d}\tau\left.\frac{\partial S(q,\tau)}{\partial\tau}\right|_{q=q(\tau)} \tag{206}$$

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where $q((\tau), p(\tau))$ are the solutions of the Hamilton equations with initial conditions $q(t_0) = q_0$ and $p(t_0) = \partial S/\partial q|_{q=q_0}$. It is convenient to choose $p(t_0) = 0$, that is, the value of $q_0 = q^*$ in which $S(q, t_0)$ has an extreme: $\partial S/\partial q|_{q=q^*} = 0$.

Appendix D. Path integral method to obtain the correlations

Let us study the RD case as an example. In order to obtain $V_0[\phi]$ from the path integral formalism we have to solve the evolution equations for $(\bar{\phi}(x,t), \pi(x,t))$ given by equation (24) with boundary conditions $(\bar{\phi}(x,-\infty), \pi(x,-\infty)) = (\phi^*(x), 0)$ and $\bar{\phi}(x,0) = \phi(x)$. The quasipotential is obtained from equation (23) by solving the Hamilton equation (22) with the RD Hamiltonian given by (12). We know that the two-body correlation $C_2(x,y)$ is related to the second derivative of the quasipotential at the deterministic stationary state (whenever V_0 is differentiable at such a point). Therefore, we want to solve the Hamilton equations when $\bar{\phi}(x,0) = \phi^*(x) + \Omega^{-1/2}\omega(x)$. We have no *a priori* guarantee that there are many paths that connect the initial condition ϕ^* at time $-\infty$ to a small deviation from it, $\bar{\phi}$. Moreover, it could also be that the path that minimizes the Lagrangian functional is one with a trajectory that travels far from the initial point. An analytic solution for these types of situations is far from our actual capabilities. Let us focus, then, on the simple assumption that the linearized dynamics correctly approximate the path that connects the initial state with the final perturbed one. As we will see, this assumption is, in practice, equivalent to the local differentiability of the quasipotential.

Let us linearize the evolution equation (24), assuming:

$$\bar{\phi}(x,t) = \phi^*(x) + \frac{1}{\sqrt{\Omega}} h[\phi^*; x]\bar{\omega}(x,t), \quad \pi(x,t) = \frac{1}{\sqrt{\Omega} h[\phi^*; x]}\bar{\eta}(x,t). \tag{207}$$

Then,

$$\begin{aligned} \partial_t \bar{\omega}(x,t) &= \int_\Lambda \mathrm{d}y\, B(x,y)\bar{\omega}(y,t) + \bar{\eta}(x,t) \\ \partial_t \bar{\eta}(x,t) &= -\int_\Lambda \mathrm{d}y\, B(y,x)\bar{\eta}(y,t) \end{aligned} \tag{208}$$

where $B(x,y)$ is defined in equation (95). The initial conditions are $(\bar{\omega}(x,-\infty), \bar{\eta}(x,-\infty)) = (0,0)$ and $\bar{\omega}(x,0) = \omega(x,0)$. The quasipotential is, in this approximation, given by:

$$V_0[\phi] = V_0[\phi^*] + \frac{1}{2\Omega}\int_{-\infty}^{0} \mathrm{d}t \int_\Lambda \mathrm{d}x\, \bar{\eta}(x,t)^2. \tag{209}$$

Let us remark that the trajectory $\bar{\eta}(x,t)$ contains the boundary conditions and therefore the $\omega(x) = \sqrt{\Omega}(\phi(x) - \phi^*(x))$ field.

$$\begin{aligned} \partial_t \bar{\omega} &= B\bar{\omega} + \bar{\eta} \\ \partial_t \bar{\eta} &= -B^{\mathrm{T}}\eta \end{aligned} \tag{210}$$

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where $\bar{\epsilon}$ and $\bar{\eta}$ are vectors and B a matrix, and B^{T} its transpose. The general solution is then

$$\begin{aligned}\bar{\eta}(t) &= \mathrm{e}^{-tB^{\mathrm{T}}}\bar{\eta}_0\\ \bar{\omega}(t) &= \mathrm{e}^{tB}a_0 + \int^t \mathrm{d}\tau\, \mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau B^{\mathrm{T}}}\bar{\eta}_0\end{aligned} \tag{211}$$

where $\bar{\eta}_0$ and a_0 are constant vectors to be determined. First, we assume that $\bar{\omega}(0) = \omega$; then,

$$\omega = a_0 + C(0)\bar{\eta}_0, \qquad C(t) = \int^t \mathrm{d}\tau\, \mathrm{e}^{-\tau B}\mathrm{e}^{-\tau B^{\mathrm{T}}} \tag{212}$$

where

$$\bar{\eta}_0 = C(0)^{-1}(\omega - a_0). \tag{213}$$

Now we assume that B can be diagonalized; that is, there exists a Q matrix such that $B = QDQ^{-1}$ with $D_{ij} = \lambda_i\delta_{i,j}$, $Q_{ij} = v_i(\lambda_j)$ where $(\lambda, v(\lambda))$ are the right eigenvalues and eigenvectors of B: $Bv(\lambda) = \lambda v(\lambda)$, $Q^{-1}_{ij} = w^*_j(\lambda_i)$ where $(\lambda^*, w(\lambda))$ are the left eigenvalues and eigenvectors of B: $B^{\mathrm{T}}w(\lambda) = \lambda^* w(\lambda)$ (a^* stands for the complex conjugate of a). Notice that the set of eigenvalues of B and B^{T} are the same. Two useful orthogonal properties can be derived from $QQ^{-1} = Q^{-1}Q = 1$:

$$w^*(\lambda_i)\cdot v(\lambda_j) = \delta_{i,j}, \quad \sum_k w^*_i(\lambda_k)v_j(\lambda_k) = \delta_{i,j}. \tag{214}$$

Observe that if B is nonsymmetric, the set of eigenvectors may not be an orthonormal vector base.

With all this information, we may introduce the boundary conditions to our general solutions. First, we see that

$$\bar{\eta}(t) = (Q^{-1})^{\mathrm{T}}\mathrm{e}^{-tD}Q^{\mathrm{T}}\bar{\eta}_0. \tag{215}$$

We know that $\bar{\eta}(-\infty) = 0$, implying that the real part of all the eigenvalues of B should be negative:

$$\mathrm{Re}(\lambda_i) < 0 \quad \forall\, i. \tag{216}$$

This is a 'stability condition' over the dynamics and it is equivalent to requiring that an arbitrary and small perturbation to the deterministic stationary state will relax to it. The second condition is $\bar{\omega}(-\infty) = 0$. Let us write the $\bar{\omega}(t)$ solution as a function of its eigenvalues:

$$\bar{\omega}\,(t) = Q\,\mathrm{e}^{tD}Q^{-1}a_0 + \int^t \mathrm{d}\tau\, Q\,\mathrm{e}^{(t-\tau)D}Q^{-1}\left(Q^{-1}\right)^{\mathrm{T}}\mathrm{e}^{-\tau D}Q^{\mathrm{T}}\bar{\eta}_0. \tag{217}$$

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First, we can show that the integral term tends to zero when $t \to -\infty$ because:

$$\left(\int^{t} \mathrm{d}\tau\, \mathrm{e}^{(t-\tau)D} Q^{-1} \left(Q^{-1}\right)^{\mathrm{T}} \mathrm{e}^{-\tau D}\right)_{ij} = -\frac{\left(Q^{-1}\left(Q^{-1}\right)^{\mathrm{T}}\right)_{ij}}{\lambda_i + \lambda_j} \mathrm{e}^{-t\lambda_j} \tag{218}$$

and we are assuming $\mathrm{Re}(\lambda_i) < 0\, \forall\, i$. On the other hand, the first term always diverges when applied to nonzero a_0 when $t \to \infty$. Therefore, $a_0 = 0$ and the solution compatible with the boundary conditions is:

$$\bar{\eta}\,(t) = \left(Q^{-1}\right)^{\mathrm{T}} \mathrm{e}^{-tD} Q^{\mathrm{T}} C(0)^{-1} \omega, \quad \bar{\omega}\,(t) = Q\, \mathrm{e}^{Dt} Q^{-1} C\,(t)\, C(0)^{-1} \omega \tag{219}$$

where

$$C(t)_{ij} = -\sum_{ks} Q_{ik} \left(Q^{-1}\left(Q^{-1}\right)^{\mathrm{T}}\right)_{ks} \left(Q^{\mathrm{T}}\right)_{sj} \frac{\mathrm{e}^{-(\lambda_k + \lambda_s)t}}{\lambda_k + \lambda_s}. \tag{220}$$

Finally, the quasipotential is:

$$\Omega V_0[\phi] = \frac{1}{2} \omega^{\mathrm{T}} \left(C(0)^{-1}\right)^{\mathrm{T}} \omega \tag{221}$$

and the two-body correlation is:

$$\bar{C} = C(0)^{\mathrm{T}} \tag{222}$$

which in the continuum limit reproduces equation (100).

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