Two refreshing views of Fluctuation Theorems through Kinematics Elements and Exponential Martingale

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Two Refreshing Views of Fluctuation Theorems Through Kinematics Elements and Exponential Martingale

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Abstract In the context of Markov evolution, we present two original approaches to obtain Generalized Fluctuation-Dissipation Theorems (**GFDT**), by using the language of stochastic derivatives and by using a family of exponential martingales functionals. We show that **GFDT** are perturbative versions of relations verified by these exponential martingales. Along the way, we prove **GFDT** and Fluctuation Relations (**FR**) for general Markov processes, beyond the usual proof for diffusion and pure jump processes. Finally, we relate the **FR** to a family of backward and forward exponential martingales.

Keywords Non-equilibrium Markov Process · Fluctuation-Dissipation Theorems · Fluctuation Relations · Martingales

1 Introduction

One of the cornerstones of statistical physics is the Fluctuation-Dissipation Theorem (**FDT**) [9, 53, 68, 80], whereby, for equilibrium systems, response to a small perturbation of the Hamiltonian is related to dynamical correlation. This theorem rationalizes the famous regression principle of Onsager [73, 74]: the decay of spontaneous fluctuation cannot be distinguished from the decay of forced fluctuation. More precisely, suppose we perturb a

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system in equilibrium at temperature T by adding to its time-independent Hamiltonian H a small time-dependent term, such that $H \to H - k_t O$. Here, O is an observable and k_t is a real function. Throughout this paper, we measure temperatures in units of the Boltzmann constant k_B. The **FDT** asserts that the response of an observable O' is related to the two-time correlation function as

$$T \frac{\delta \langle O'_t \rangle'}{\delta k_s}\bigg|_{k=0} = \partial_s \langle O_s O'_t \rangle, \tag{1}$$

with $t \geq s$. In this relation, the brackets, $\langle\ \rangle$ and $\langle\ \rangle'$, denote expectation in the unperturbed and perturbed processes, respectively. Since mid-nineties, this theorem has been extended to nonequilibrium systems in two related directions. The first is the discovery of various Fluctuation Relations (**FR**) [19, 32, 35, 49], the so-called **Gallavotti-Cohen relation** [32, 35], the **Jarzynski equality** [49] and the **Crooks theorem** [19]. All of these hold arbitrarily far from equilibrium and can be viewed as non-perturbative extensions [36] of the **FDT** (1). These relations constrain the distribution of entropy production or work performed in the system. The second is the extension of the relation (1) between response and correlation in the linear response regime to nonequilibrium states (stationary as well as non-stationary), for example, those in glassy systems and soft spin models [18, 20, 27, 60, 69] and also in relation to broken supersymmetry [91]. This second direction has seen an upsurge in the last three years through formulation of the Generalized Fluctuation-Dissipation Theorems (**GFDT**), mainly in the works of Seifert and Speck in Stuttgart [83, 85, 86], Baiesi, Maes and Wynants in Leuven [3, 4, 67], and Gawedzki and Chetrite in Lyon and Falkovich in Rehovot [12–14] (see, also, the works [64, 78]). Moreover, experimental verifications of the **GFDT** on colloidal particle have been done in Lyon [38, 39].

In the present paper, we revisit, generalize, and unify these **FR** and **GFDT** by couching them in the language of the kinematics of a general Markov process, without strict mathematical rigor. We show that this language allows elementary proofs and generalizations of the different **GFDT** which exist in the literature. We also consider a new family of non-perturbative extensions of the **GFDT** which concerns a so-called **exponential forward martingale** functionals [16, 76, 79]. Finally, we revisit the **FR** and show their relation to forward and backward exponential martingales.[1] In the process, we prove that a certain version of the Crooks theorem and the Jarzynski equality hold for fairly general Markov processes, whereas the Gallavotti-Cohen relation for the performed work can be violated when the particle is subjected to a Poisson or Levy noise [6, 89].

General Markov stochastic processes form an integral part of modeling of dynamics in statistical mechanics. Although largely idealized, they often provide a sufficiently realistic description of experimental situations and have traditionally served as a playground for both theoretical considerations and numerical studies. In a continuous space (e.g., $\mathscr{R}^d$), all continuous time Markov processes consist of some combinations of diffusion, deterministic motion and random jumps. Markov processes corresponding to equilibrium dynamics are characterized by the detailed balance property which ensures that the net probability flux between microstates of the system vanishes. On the other hand, with nonequilibrium Markov dynamics, detailed balance is violated and there are non-zero probability fluxes even in a stationary situation. For the purpose of characterizing the difference between equilibrium and nonequilibrium dynamics, it is interesting to find a vector field, a kind of velocity, which vanishes in equilibrium. Such an object was introduced in the sixties by Nelson in his seminal work [71] with the notion of current velocity that we call here the **local symmetric**

[1] In the following, unless stated otherwise, use of the word martingale alone would mean forward martingale.

velocity. This quantity is an average of a well-chosen instantaneous velocity of the process conditioned to pass through a given point. It was shown in [14] that nonequilibrium diffusive dynamics (without the random jumps) takes, in the Lagrangian frame of this velocity, an equilibrium form with the detailed balance property and this explains the usual form (1) of the **FDT** in that frame, which was observed previously in [12]. The issue regarding the extension of this result to other types of Markov processes is addressed in this article in one of the Sections.

The formulation of the usual **FDT** (1) for some Markov processes is known since long time [9, 53, 80] in physics, but now it has a strictly mathematically rigorous formulation [25]. For the **FR**, shortly after the earliest articles in the context of deterministic dynamics [32, 35], the fluctuation relations were proved for some Markovian dynamics. In [50], Jarzynski generalized his relation to time-dependent pure jump Markov processes. At around the same time, Kurchan showed in [57] that the stationary **FR** hold for the stochastic Langevin-Kramers evolution with additive noise. His result was extended to more general diffusion processes by Lebowitz and Spohn in [59]. In [66], Maes has traced the origin of **FR** to the Gibbsian nature of the statistics of the dynamical histories. Finally, these relations were put into the language of stochastic thermodynamics by Sekimoto [84] and Seifert [82]. There exist now many reviews on fluctuation relations in the Markovian context, like [42, 51, 63] for pure jump process or [10, 11, 51, 58, 62] for diffusion process, but the extension to **FR** for general Markov process is still under debate [6, 89].

The paper consists of seven Sections and six Appendices. Section 2 sets the stage and provides notations by briefly stating definitions relevant to Markov processes. In particular, in Sect. 2.1, we recall the notions of transition probability, Markov generator, stationary state and equilibrium state. In Sect. 2.2, we introduce the notion of cotransition probability, cogenerator, current and velocity operator. We also elucidate the relation between these objects. Section 3 develops the kinematics of a Markov process [71] by defining a set of local derivatives and local velocities associated with such processes. It is proved in Sect. 3.2 that these local derivatives appear naturally in the time derivative of correlation function which appears on the right hand side of the **FDT** (1). Section 4 investigates the form of the kinematics elements, local velocities and velocity operator, for the three most common examples of Markov process which appear in physics. First is the pure jump process in Sect. 4.1, which is a process with no diffusion and deterministic evolution. Second is the diffusion process, considered in Sect. 4.2, which is a process that, on the contrary, neglects the random jumps. Finally, in Sect. 4.3, we investigate the less considered case which mixes diffusion, random jumps and deterministic motion given by a stochastic equation with Gaussian and Poissonian white noises. The latter noise consists of a sequence of δ-function shaped pulses with random heights occurring at randomly distributed times. Such a noise appears in the physical world, for example, it describes the emission of electrons in diodes or the counting process of photons. As examples, we study two physical realizations of such a dynamics involving colloidal particles trapped on the unit circle. It turns out that analytical computation of the stationary density is possible only for the first realization, and not for the second. Hence, we resort to extensive numerical simulations to obtain the stationary density as well as the local velocity for the second realization.

The first central section which contains novel results is Sect. 5 which is devoted to the study of the behavior of a Markovian system under a perturbation. More precisely, Sect. 5.1 recalls the notion of response function to an arbitrary perturbation. Section 5.2 introduces a special family of perturbations, which we call Hamiltonian ones or generalized Doob h-transforms. These include the usual perturbations considered in the physics literature. Section 5.3 proves in a very simple way, thanks to the language of kinematics elements, that the recent **GFDT** [3, 4, 12–14, 38, 64, 67, 78, 83, 85, 86] are obtained in this general Markovian context for the case of a Hamiltonian perturbation. We also numerically verify the **GFDT** in the context of the example of Sect. 4.3.2 involving stochastic dynamics with Gaussian and Poissonian white noise. Section 5.4 presents the **GFDT** which result from a more general class of perturbations, such as a time change [25] or a thermal perturbation pulse [14, 80]. The second crucial section is Sect. 6. Here, we present global (non-perturbative) versions of these **GFDT** which involve a family of functionals called exponential martingales in the probability literature [76]. Originally, a martingale referred to a class of betting strategies, but this notion has now become central to the modern probability theory and characterizes, ironically, a model of a fair game. A martingale is process whose expectation in the future, given the knowledge accumulated up to now, is its present value [16, 28, 33, 79, 87]. In Sect. 6.1, we present a family of exponential martingales, which are natural objects associated with the Hamiltonian perturbations because they are the ratio of the trajectory measures of the perturbed and the unperturbed processes. Moreover, we prove in Sect. 6.1.3 that they also provide global versions of the GFDT. Finally, in Sect. 6.2, we revisit, in the light of the martingale theory, the usual **FR** for quite general Markov processes and underline the relation with the previously considered exponential martingales. In particular, this rationalizes the typical martingale form $\langle \exp(-W)\rangle = 1$ of the Jarzynski equality. Section 7 presents our conclusions. The Appendices collect some simple but technical arguments.

2 Elements of a Markov Process

As mentioned in the introduction, our study deals with nonequilibrium systems modeled by Markov processes. We begin by recollecting below some basic properties of a Markov process [2, 7, 16, 28, 33, 79, 87]. We consider a continuous time Markov process $\mathbf{x}_t$ which takes values in a space $\mathscr{E}$. The space $\mathscr{E}$ could, for example, be $\mathscr{R}^d$ or a counting space.

2.1 Transition Probability, Stationary State and Equilibrium

The dynamics of the process is given by a family of transition functions[2] $P_s^t(x, dy)$ which satisfy the Chapmann-Kolmogorov rule:

$$\int P_s^u(x, dy) P_u^t(y, dz) = P_s^t(x, dz) \quad \forall s \le u \le t, \tag{2}$$

where $P_s^u(x, dy)$ is the probability that the process has the value $[y, y + dy]$ at time u, conditioned on the fact that it had the value x at time s. Here, and in the following, the notation dy represents the Lebesgue measure or the counting measure, depending on $\mathscr{E}$. We will assume for simplicity that the transition functions and all other relevant functions admit a density with respect to this measure (i.e., $P_s^t(x, dy) = P_s^t(x, y)dy$). Moreover, we consider processes without death or explosion, i.e., with so-called honest transition probabilities, such that one has the normalization condition $\int dy P_s^t(x, y) = 1$. This could be easily achieved in general, e.g., by enlarging the space to include a coffin state. It will be useful to think of the

[2]Presence of two time indices is a result of the non-homogeneous time character of the process. Such a process is sometimes called nonstationary in physics. For time-homogeneous process, we define $P_{t-s} \equiv P_s^t$.

transition functions as linear operators P_s^t which form an inhomogeneous semi-group, and which are defined by their action on a bounded function f in $\mathscr{E}$ in the following way:

$$P_s^t[f](x) \equiv \int dy\, P_s^t(x,y) f(y). \tag{3}$$

The family of transition functions of a Markov process which can be written down explicitly is very restrictive. Hence, it is more practical to define the generator L_t of this inhomogeneous semi-group, under appropriate regularity conditions [16, 79], by the following equation:

$$P_s^t = \overrightarrow{\exp}\left(\int_s^t L_u\, du\right) \equiv \sum_n \int_{s\le s_1\le s_2\le\cdots\le s_n\le t} \prod_{i=1}^n ds_i\, L_{s_1}\circ L_{s_2}\circ\cdots\circ L_{s_n}. \tag{4}$$

This equation is equivalent to the forward and backward Kolmogorov equation, given, respectively, by

$$\partial_t P_s^t = P_s^t \circ L_t, \quad \text{and} \quad \partial_s P_s^t = -L_s \circ P_s^t. \tag{5}$$

Here, the symbol $\circ$ means composition of operators. Also, the initial condition is $P_s^s = \mathscr{I}$. For the transition function to be honest, the generator must obey $L_t[1] = 0$, where 1 is the function which is equal to 1 on $\mathscr{E}$. If the initial measure of the process is $\mu_0(dx) = \rho_0(x)dx$, we may define the averages of a functional of the process $\mathbf{x}$ as

$$\langle F\rangle \equiv \int \mu_0(dx)\mathbf{E}_{t_0,x}(F[x]), \tag{6}$$

where $\mathbf{E}_{t_0,x}$ stands for the expectation of the functional of the process $\mathbf{x}$ with the initial condition $x_{t_0} = x$. Next, it will be useful to define a path measure $M_{\mu_0,[s,t]}[dx] \equiv dM_{\mu_0,[s,t]}[x]$ on the space of trajectories by the following equation:

$$\langle F\rangle = \int F[x]\, M_{\mu_0,[s,t]}[dx], \tag{7}$$

where F is a functional of the path from time s to time t. The instantaneous (or single time) probability density function (PDF) of the process is given by

$$\rho_t(x) = \langle \delta(x_t - x)\rangle. \tag{8}$$

Its time evolution may be deduced from (5). We obtain the following Fokker-Planck equation:

$$\partial_t \rho_t = L_t^\dagger[\rho_t], \tag{9}$$

where $L_t^\dagger$ is the formal adjoint of L_t with respect to the Lebesgue (or counting) measure. A **stationary state** ($\rho_t \equiv \rho$) then satisfies the equation

$$L_t^\dagger[\rho] = 0. \tag{10}$$

Further, one says that the process is in equilibrium, i.e., it satisfies the infinitesimal detailed balance relation if the following condition for the generator is satisfied:[3]

$$\rho \circ L_t \circ \rho^{-1} = L_t^{\dagger}. \tag{11}$$

If the process is time-homogeneous, the above equation is equivalent to the usual detailed balance condition for the transition function:

$$\rho(x) P_{t-s}(x, y) = \rho(y) P_{t-s}(y, x). \tag{12}$$

It will be useful to define two particular families of non-stationary states. First, one defines the so-called accompanying density π_t which satisfies the instantaneous relation [41, 50]

$$L_t^{\dagger}[\pi_t] = 0. \tag{13}$$

Next, we introduce the subclass of accompanying density, that we assume to be in local detailed balance, such that the generator verifies the instantaneous time-dependent version of the relation (11):

$$\pi_t \circ L_t \circ \pi_t^{-1} = L_t^{\dagger}. \tag{14}$$

2.2 Cotransition Probability, Current and Velocity Operator

The two-point density $\langle \delta(x_s - x)\delta(x_t - y)\rangle$ of a Markov process is usually expressed by conditioning with respect to the earlier time s, as

$$\langle \delta(x_s - x)\delta(x_t - y)\rangle = \rho_s(x) P_s^t(x, y). \tag{15}$$

It can also be expressed by conditioning with respect to the later time t in terms of the so-called cotransition probability P_s^{*t} [30] (sometimes called the backward transition probability [31, 72][4]) as

$$\langle \delta(x_s - x)\delta(x_t - y)\rangle = P_s^{*t}(x, y)\rho_t(y). \tag{16}$$

This cotransition probability satisfies the Chapman-Kolmogorov equation (2), but the normalization condition becomes $\int dx\, P_s^{*t}(x, y) = 1$. The relation between the transition and the cotransition probability can then be expressed by the operator formula $P_s^{*t} = \rho_s \circ P_s^t \circ \rho_t^{-1}$, which implies the forward equation[5]

$$\partial_t P_s^{*t} = P_s^{*t}\left(\rho_t \circ L_t \circ \rho_t^{-1} - \rho_t^{-1}(\partial_t \rho_t)\right). \tag{17}$$

We will now introduce a family of operators L_t^*, which we call cogenerators, by the following equation:

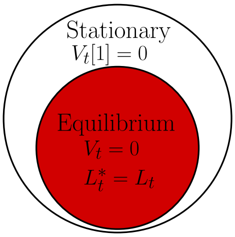
$$L_t^* = \rho_t^{-1} \circ L_t^{\dagger} \circ \rho_t - \rho_t^{-1}(\partial_t . \rho_t)\mathscr{I} = \rho_t^{-1} \circ L_t^{\dagger} \circ \rho_t - \rho_t^{-1} L_t^{\dagger}[\rho_t]\mathscr{I}, \tag{18}$$

[3] Note that, with this definition, a non-homogeneous process can be in equilibrium. We will see examples of diffusion process with this surprising property in Sect. 4.2.

[4] We will not employ this terminology because in our language, the backward process needs also a reversal of time [11].

[5] Here, the density ρ is regarded as a multiplication operator. In the following, depending on the context, we will consider ρ as a function or as an operator.

Fig. 1 The figure illustrates the relation between stationarity, equilibrium and the condition $L_t^* = L_t$, as discussed in the text



where $\mathscr{I}$ is the identity kernel, so that the cotransition probability now takes the operatorial form

$$P_s^{*t} \equiv \overrightarrow{\exp}\left(\int_s^t du\, \left(L_u^*\right)^\dagger\right). \tag{19}$$

Then, the property $\int dx\, P_s^{*t}(x, y) = 1$ is equivalent, as before, to $L_t^*[1] = 0$. For a stationary process (10), the cogenerator takes the form $L_t^* = \rho^{-1} \circ L_t^\dagger \circ \rho$, which is the adjoint of L_t with respect to the scalar product with weight ρ. It is also interesting to associate a **current operator** and a **velocity operator** (which depend on the initial density) with the density ρ_t by the following equations:

$$J_t \equiv \rho_t \circ L_t - L_t^\dagger \circ \rho_t \quad \text{and} \quad V_t \equiv L_t - \rho_t^{-1} \circ L_t^\dagger \circ \rho_t. \tag{20}$$

The Fokker-Planck equation (9) can be expressed as

$$\partial_t \rho_t + J_t[1] = 0, \quad \text{or, equivalently,} \;\; \partial_t \rho_t + \rho_t V_t[1] = 0. \tag{21}$$

The condition (10) for the density ρ to be stationary can then be expressed as

$$J_t[1] = 0, \quad \text{or, equivalently,} \;\; V_t[1] = 0. \tag{22}$$

Otherwise, the equilibrium condition (11) becomes

$$J_t = 0, \quad \text{or, equivalently,} \;\; V_t = 0. \tag{23}$$

Finally, using (9,18,20), we can express the cogenerator in terms of the velocity operator as

$$L_t^* = L_t - V_t + V_t[1]\mathscr{I}. \tag{24}$$

Then, by (24), equilibrium implies $L_t^* = L_t$. The converse of this statement is true because the condition $L_t^* = L_t$ implies that for any function f, one has $L_t^\dagger[\rho_t f] - f L_t^\dagger[\rho_t] = \rho_t L_t[f]$. Then, on integrating by parts over all space, we get $\int dx(-2f(x)L_t^\dagger[\rho_t](x)) = 0$, which implies that $L_t^\dagger[\rho_t] = 0$, and then $\rho_t = \rho$. Finally, the condition $L_t^* = L_t$ can be rewritten as the equilibrium condition.

Figure 1 illustrates these relations between stationarity, equilibrium and the condition of equality between the generator and the cogenerator.

3 Kinematics of a Markov Process

The notion of the velocity operator (20) introduced in the last section is quite different from the usual notion of velocity as the derivative of the position. Assume that we want to describe the "naive" kinematics of a general Markov process. The first difficulty is that the trajectories in general are non-differentiable (as in a diffusion process) or, worse, discontinuous (as in a jump process). This does not allow for a straightforward definition of a velocity. In the sixties, Nelson circumvented this difficulty by introducing the notion of forward and backward **stochastic derivatives** in his seminal work concerning diffusion process with additive noise [71]. Here, we will reproduce the definition of Nelson for a general Markov process. In the following, we assume existence conditions on various quantities, with the expectation that these conditions have already been, or, can be established by rigorous mathematical studies.

3.1 Stochastic Derivatives, Local Velocity

According to Nelson, a Markov process is said to be mean-forward differentiable if the limit

$$\frac{\lim_{h\to 0}\langle \frac{x_{t+h}-x_t}{h}\delta(x_t-x)\rangle}{\langle\delta(x_t-x)\rangle}$$

exists. In this case, this ratio defines the local forward velocity for a process conditioned to be in x at time t:

$$v_t^+(x)\equiv\frac{\lim_{h\to 0}\langle \frac{x_{t+h}-x_t}{h}\delta(x_t-x)\rangle}{\langle\delta(x_t-x)\rangle}. \tag{25}$$

Similarly, the local backward velocity is defined as

$$v_t^-(x)\equiv\frac{\lim_{h\to 0}\langle \frac{x_{t}-x_{t-h}}{h}\delta(x_t-x)\rangle}{\langle\delta(x_t-x)\rangle}. \tag{26}$$

The local symmetric velocity and the local osmotic velocity are defined as

$$v_t(x)\equiv\frac{v_t^+(x)+v_t^-(x)}{2}\quad\text{and}\quad o_t(x)\equiv\frac{v_t^+(x)-v_t^-(x)}{2}. \tag{27}$$

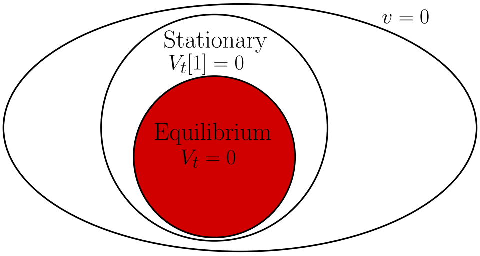
In the same spirit, he defined the stochastic forward, backward and symmetric derivatives of function $f_t(x_t)$ of the process as

$$\begin{cases}\frac{d_+f}{dt}(x)\equiv\frac{\lim_{h\to 0}\langle\frac{f(t+h,x_{t+h})-f(t,x_t)}{h}\delta(x_t-x)\rangle}{\langle\delta(x_t-x)\rangle},\\ \frac{d_-f}{dt}(x)\equiv\frac{\lim_{h\to 0}\langle\frac{f(t,x_t)-f(t-h,x_{t-h})}{h}\delta(x_t-x)\rangle}{\langle\delta(x_t-x)\rangle},\\ \frac{df}{dt}(x)\equiv\frac{\frac{d_+f}{dt}(x)+\frac{d_-f}{dt}(x)}{2}.\end{cases} \tag{28}$$

Note that the set of forward, backward and symmetric local velocities are just special cases of derivatives of the function $f_t(x_t)=x_t$. With the definition of the forward transition probability and the cotransition probability given in (15) and (16), we can rewrite the above equations as

$$\begin{cases}\frac{d_+f}{dt}(x)=\lim_{h\to 0}\frac{1}{h}\int dy\,P_t^{t+h}(x,y)(f(t+h,y)-f(t,x)),\\ \frac{d_-f}{dt}(x)=\lim_{h\to 0}\frac{1}{h}\int dy\,P_{t-h}^{*t}(y;x)(f(t,x)-f(t-h,y)).\end{cases} \tag{29}$$

Fig. 2 The figure illustrates the relation between stationarity, equilibrium, and vanishing of the local symmetric velocity, as discussed in the text



A Taylor expansion of these transition probabilities using (4) and (19) gives

$$\frac{d_+}{dt} = \partial_t + L_t \quad \text{and} \quad \frac{d_-}{dt} = \partial_t - L_t^*. \tag{30}$$

Also, the stochastic symmetric derivative becomes

$$\frac{d}{dt} = \partial_t + \frac{L_t - L_t^*}{2}. \tag{31}$$

The expression of the cogenerator from (24) allows us to express the stochastic symmetric derivative in (31) in terms of the velocity operator (20) as

$$\frac{d}{dt} = \partial_t + \frac{V_t - V_t[1]\mathscr{I}}{2}. \tag{32}$$

Then, for a steady state (22), $\frac{d}{dt} = \partial_t + \frac{V_t}{2}$.

We can then deduce that, in the equilibrium case, the stochastic symmetric derivative takes the form of the partial time derivative $\frac{d}{dt} = \partial_t$, which gives zero while acting on observables which do not depend explicitly on time. The local symmetric velocity, given in (27), now reads

$$v_t^i(x) = \frac{L_t[x] - L_t^*[x]}{2} = \frac{V_t[x^i] - V_t[1]x^i}{2}, \tag{33}$$

and then, for a steady state, $v_t^i(x) = \frac{V_t[x^i]}{2}$.

It is important to remark that equilibrium ($V = 0$) implies vanishing of the local symmetric velocity but the converse of this statement is not true. Figure 2 illustrates the relation between stationarity, equilibrium and vanishing of the local symmetric velocity.

One of the authors of the present article proved in [14] that a diffusion process in the Lagrangian frame of its mean local symmetric velocity takes an equilibrium form, and then the concept of equilibrium and nonequilibrium become closer than usually perceived. However, this property is no longer true for a general process due to the inequivalence between equilibrium and vanishing of the local symmetric velocity.

3.2 Time Derivative of Two-point Correlations

Here we provide useful formulae for the time derivative of the two-time ($s \leq t$) correlation of observables U and V in terms of the correlation of stochastic derivatives (forward or backward) of these observables. The two-point correlation can be expressed in term of the forward transition probability and cotransition probability, (15), (16), as

$$\langle U_s(x_s)V_t(x_t)\rangle = \int dxdy U_s(x)\rho_s(x)P_s^t(x,y)V_t(y) = \int dxdy U_s(x)P_s^{*t}(x,y)\rho_t(y)V_t(y). \tag{34}$$

We then obtain the formula

$$\partial_t\langle U_s(x_s)V_t(x_t)\rangle = \left\langle U_s(x_s)\frac{d_+V_t}{dt}(x_t)\right\rangle \quad \text{and} \quad \partial_s\langle U_s(x_s)V_t(x_t)\rangle = \left\langle \frac{d_-U_s}{ds}(x_s)V_t(x_t)\right\rangle. \tag{35}$$

The proofs are direct consequence of the definition of transition and cotransition probabilities (4, 19) and of forward and backward stochastic derivatives, and are given in Appendix A. These relations provide motivation for a proof of generalizations of **FDT** by involving the stochastic derivatives, as discussed later in the paper.

4 Examples of Markov Processes

We will now investigate the form of the velocity operator (20) and of the local symmetric velocity (33) for the three most popular examples of Markov processes, namely, the pure jump process, the diffusion process and a process generated by a stochastic equation with both Gaussian and Poissonian white noise.

4.1 Pure Jump Process

Roughly speaking, a Markov process is called a pure jump process (or, a pure discontinuous process) if, after "arriving" into a state, the system stays there for an exponentially-distributed random time interval. It then jumps into another state chosen randomly, where it spends a random time, and so on. More precisely, $\mathbf{x}_t$ is a pure jump process if, during an arbitrary time interval $[t, t+dt]$, the probability that the process undergoes one unique change of state (respectively, more that one change of state) is proportional to dt (respectively, infinitesimal with respect to dt) [33]. In a countable space, one can show that all Markov processes (with right continuous trajectories) are of this type, a property which is not true in a general space. It is usual to introduce the intensity function $\lambda_t(x)$ such that $\lambda_t(x)dt + o(\lambda_t(x)dt)$ is the probability that $\mathbf{x}_t$ undergoes a random change in the time interval $[t, t+dt]$ if the actual state is $x_t = x$. If this change occurs, then $x(t+dt)$ is distributed with the transition matrix $T_t(x, dy)$. Such a process naturally generalizes a Markov chain to continuous time.

We introduce the transition rate of the jump process, which gives the rate at time t for the transition $x \to y$, through

$$W_t(x, dy) \equiv \lambda_t(x)T_t(x, dy). \tag{36}$$

One can prove that, with regularity condition [33, 79], such a process possesses the generator

$$L_t(x, y) = W_t(x, y) - \delta(x-y)\left(\int dz W_t(x, z)\right). \tag{37}$$

The current and the velocity operator, given in (20), take the form of the kernel

$$\begin{aligned} &J_t(x, y) = \rho_t(x)W_t(x, y) - W_t(y, x)\rho_t(y) \\ &\text{and} \\ &V_t(x, y) = W_t(x, y) - \rho_t^{-1}(x)W_t(y, x)\rho_t(y). \end{aligned} \tag{38}$$

Otherwise, the local symmetric velocity (33) takes the form

$$v_t(x) = \frac{1}{2}\int V_t(x, y)(y - x)dy. \tag{39}$$

4.2 Diffusions Processes

Here we are interested in a Markov process which has continuous trajectories. More concretely, the main objects of our study are the non-autonomous stochastic processes $\mathbf{x}_t$ in $\mathscr{R}^d$ (or, more generally, on a d-dimensional manifold), described by the differential equation

$$\dot{x} = u_t(x) + \eta_t(x), \tag{40}$$

where $\dot{x} \equiv \frac{dx}{dt}$, $u_t(x)$ is a time-dependent deterministic vector field (a drift), and $\eta_t(x)$ is a Gaussian random vector field with mean zero and covariance

$$\left\langle \eta_t^i(x)\eta_s^j(y)\right\rangle = \delta(t-s)D_t^{ij}(x, y). \tag{41}$$

Due to the white-noise nature of the temporal dependence of η_t (typical η_t are distributional in time), (40) is a stochastic differential equation (SDE). We shall consider it with the Stratonovich convention [87], keeping for the Stratonovich SDE's the notation of the ordinary differential equations (ODE's). The explicit form of generator L_t which acts on a function f is

$$L_t[f] = \widehat{u}_t^i \partial_i f + \tfrac{1}{2}\partial_j \left[d_t^{ij}\partial_i f\right], \tag{42}$$

where

$$d_t^{ij}(x) = D_t^{ij}(x, x) \quad \text{and} \quad \widehat{u}_t^i(x) = u_t^i(x) - \tfrac{1}{2}\partial_{y^j} D_t^{ij}(x, y)|_{y=x}. \tag{43}$$

Here, $\widehat{u}_t^i(x)$ is called the modified drift. A particular form of (40) which is very popular in physics is the so-called overdamped Langevin form (with the Einstein relation):

$$\dot{x}^i = -\Gamma_t^{ij}(x)\partial_j H_t(x) + G_t^i(x) + \frac{1}{2}\partial_{y^j} D_t^{ij}(x, y)\bigg|_{x=y} + \eta_t^i(x) \quad \text{and} \quad d_t^{ij}(x) = \frac{2}{\beta}\Gamma_t^{ij}(x), \tag{44}$$

where $H_t(x)$ is the Hamiltonian of the system (the time index corresponds to an explicit time dependence), $\Gamma_t(x)$ is a family of non-negative matrices, $G_t(x)$ is an external force (or a shear), β the reciprocal of the bath temperature and $\partial_{y^j} D_t^{ij}(x, y)|_{x=y}$ is an additional spurious term which comes from the x dependence of the noise. This additional term is chosen in such a way that the accompanying density (13) is the Gibbs density $\frac{\exp(-\beta H_t)}{Z_t}$, in the case where the external force is zero ($G = 0$). Then, in the case of stationary Hamiltonian and temperature (i.e., $H_t = H, \beta_t = \beta$) and without the external force (i.e., $G = 0$), the Gibbs density $\frac{\exp(-\beta H)}{Z}$ is an equilibrium density, see (11). Note that this last case, in the situation where the matrix Γ_t depends explicitly on time, is an example of a non-homogeneous process in equilibrium in the state $\exp(-\beta H)$. The presence of the spurious term $\partial_{y^j} D_t^{ij}(x, y)|_{x=y}$ was extensively studied in the literature of non-linear Brownian motion [55] and we can see that it vanishes in the case of linear Brownian motion where

$\Gamma_t(x) = \Gamma_t$. The overdamped property comes from neglect of the Hamiltonian forces.[6] In addition to the operator current, the operator velocity (20) and the local symmetric velocity (33), it is usual for this type of process to introduce the hydrodynamic probability current j_t, respectively, the **hydrodynamic velocity** $\widetilde{v}_t$, associated with the PDF ρ_t, (8), through

$$j_t = \widehat{u}_t \rho_t - \frac{d_t}{2}(\nabla \rho_t) \quad \text{and} \quad \widetilde{v}_t = \widehat{u}_t - \frac{d_t}{2}(\nabla \ln \rho_t), \tag{45}$$

such that the Fokker-Planck equation (9) takes the form of the continuity equation, respectively, the hydrodynamical advection equation,

$$\partial_t \rho_t + \nabla_i j_t^i = 0 \quad \text{and} \quad \partial_t \rho_t + \nabla_i \left(\rho_t \widetilde{v}_t^i\right) = 0. \tag{46}$$

A direct calculation, given in Appendix B, shows that the explicit form of the cogenerator (18) for a diffusion process is

$$L_t^*[f] = L_t[f] - 2\widetilde{v}_t.\nabla f, \tag{47}$$

and we can deduce the form of the operator velocity, (20), as

$$\begin{aligned} V_t[f] &= \left(L_t - \rho_t^{-1} \circ L_t^\dagger \circ \rho_t\right)[f] \\ &= \left(L_t - L_t^* - \rho_t^{-1}(\partial_t.\rho_t)\mathcal{I}\right)[f] = 2\widetilde{v}_t.\nabla f + \left(\rho_t^{-1}\nabla_i\left(\rho_t \widetilde{v}_t^i\right)\right) f. \end{aligned} \tag{48}$$

Moreover, for a diffusion process, (47) allows us to obtain the following hydrodynamical form for the stochastic symmetric derivative and the local symmetric velocity.

$$\frac{d}{dt} = \partial_t + \widetilde{v}_t.\nabla \quad \text{and} \quad v_t(x) = \widetilde{v}_t(x). \tag{49}$$

It then follows that the local symmetric velocity is identical to the hydrodynamic velocity, and moreover, with (48), that the equilibrium condition ($V_t = 0$) is equivalent to the condition of vanishing of the hydrodynamic velocity $\widetilde{v}_t$ or the local symmetric velocity in $\mathscr{E}$.[7] Also, the form of the drift of an equilibrium diffusion is then

$$\widehat{u}_t = \frac{d_t}{2}(\nabla \ln \rho). \tag{50}$$

The link between stationarity, equilibrium and vanishing of local symmetric velocity for a diffusion process is depicted in Fig. 3.

4.3 Stochastic Equation with Gaussian and Poissonian White Noise

We now consider a Markov process in continuous space (e.g., $\mathscr{R}^d$) which includes the processes in the last two sections in the sense that both diffusion and jump can occur. Such processes are very popular in finance [17, 70]. They are much less popular in physics, where,

[6] The Fluctuation-Dissipation Theorem with such Hamiltonian force has been studied in details in [13, 14].

[7] In [22], a result in a similar spirit was shown for the characterization of diffusion processes with additive covariance $d_t^{ij}(x) = d\delta^{ij}$ which possesses a (possibly time-dependent) gradient drift. The characterization can be written in terms of a second-order stochastic derivative as $\frac{d_+ d_+ x_t}{dt^2} = -\frac{d_- d_- x_t}{dt^2}$.

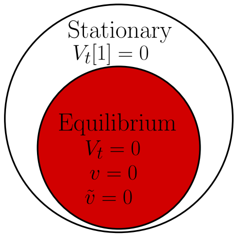


Fig. 3 The set of processes inside the domain marked in red are such that the local symmetric velocity vanish, but it is also the set of equilibrium jump processes and the set of processes with vanishing hydrodynamic velocity

after its first study in the beginning of eighties [40, 90], they were used, for example, to study mechanism of noise-induced transitions [81] or noise-driven transport [21, 65]. We consider processes that are right continuous with a left limit (i.e., "cadlag" processes), and we define $x_{t^-} = \lim_{s\uparrow t} x_s$ and the jump as

$$\Delta x_t = x_t - x_{t^-}. \tag{51}$$

We want to consider a process which follows the evolution of a diffusion process (40) for most of the time, excepting that it jumps occasionally, the occurrence of the jump being given by a non-autonomous Poisson process. More precisely, we will construct such processes by adding a state-dependent Poisson noise [77] to the stochastic differential equation (40), as

$$\dot{x}_t = u_t(x_t) + \eta_t(x_t) + w_t(x_{t^-}), \tag{52}$$

where, as before, $\eta_t(x)$ is a Gaussian random vector field (with Stratonovich convention [87]) which has mean zero and covariance (41). On the other hand, $w_t(x)$ is a state-dependent Poisson noise (that depends on the state x_t), and is given by

$$w_t(x) = \sum_{i=1}^{N_t} y_i(x)\delta(t - T_i). \tag{53}$$

The time T_i at which the instantaneous jump occurs are the arrival times of a non-homogeneous and non-autonomous Poisson process N_t with intensity $\lambda_t(x)$. The jump magnitude y_i are mutually-independent random variables, independent of the Poisson process, and are described by the probability function $b_{t,x}(y)$. This function gives the probability for a jump of magnitude y while starting from x at time t. Physically, addition of the Poisson noise mimics large instantaneous inflows or outflows ("big impact") at the microscopic level. We remark that this noise contains almost surely a finite number of jumps in every interval ($\lambda_t(x)$ is finite). It is possible to consider a more general noise, the so-called Levy noise, where this condition is relaxed.[8] The mathematical theory of general stochastic differential

[8]The process $\mathbf{x}_t$ then describes a fairly large class of Markov processes (of Feller-type) which are governed by Levy-Ito generators which acts on a function f as the integro-differential operators [46–48, 88]

$$L_t[f](x) = \widehat{u}_t^i(x)\partial_{x^i} f + \frac{1}{2}\partial_{x^j}\left[d_t^{ij}(x)\partial_{x^i} f\right] + \int_{\mathscr{R}^d-\{0\}}\left(f(x+y) - f(x) - \frac{(y.\nabla f)(x)}{1+|y|^2}\right)\nu_{t,x}(dy), \tag{54}$$

with the so-called Levy jump measure $\nu_{t,x}(dy)$ which can be infinite but is such that, for all x and t, the condition $\int_{\mathscr{R}^d-\{0\}} \frac{|y|^2}{1+|y|^2}\nu_{t,x}(dy) < \infty$ is verified.

equation with a Levy noise and the theory of stochastic integration with respect to a (possibly discontinuous) more general (semi- martingale) noise are well established [2, 5]. In the present case, we will just use from this theory the form of the Markov generator which, for the process (52), is an integro-differential operator, given by

$$L_t = L_t^D + L_t^J. \tag{55}$$

Here, the diffusive part L_t^D is given by (42) and the jump part L_t^J is given by (37), with

$$W_t(x, y) = \lambda_t(x) b_{t,x}(y - x). \tag{56}$$

The class of process (52) possesses some famous particular cases.

– The piecewise deterministic process [23] is the case where there is no Gaussian noise ($\eta_t(x) = 0$). Then x_t follows a deterministic trajectory interrupted by jumps of random timing and amplitudes.
– The interlacing Levy Processes [2] is the case where the drift is constant and homogeneous ($u_t(x_t) = u$), the Gaussian noise is additive and stationary ($d_t^{ij}(x) = d^{ij}$), and the Poisson white noise is state-independent and stationary ($\lambda_t(x_t) = \lambda$ and $b_{t,x}(y) = b(y)$). This process belongs to the class of Levy process [2], with independent and homogeneous increments.

We will now investigate the form of the kinematics elements: the velocity operator, (20), and the local symmetric velocity, (33). Similar to (55), these two objects can be split into a diffusive part and a jump part such that

$$V_t = V_t^D + V_t^J \quad \text{and} \quad v_t = v_t^D + v_t^J. \tag{57}$$

On using (178), we can express the diffusive part V_t^D as (48)

$$\begin{aligned} V_t^D &\equiv L_t^D - \rho_t^{-1} \circ L_t^{D,\dagger} \circ \rho_t \\ &= \rho_t^{-1} \nabla_i \left(\rho_t \left(\widehat{u}_t^i - \frac{d_t^{ij}}{2} (\nabla_j \ln \rho_t) \right) \right) + 2 \left(\widehat{u}_t^i - \frac{d_t^{ij}}{2} (\nabla_j \ln \rho_t) \right) \nabla_i. \end{aligned} \tag{58}$$

The jump part V_t^J is given by (38) with (56). Similarly, the diffusive part of the local symmetric velocity reads

$$v_t^D(x) = \widehat{u}_t^i(x) - \frac{d_t^{ij}(x)}{2} \left(\nabla_j \ln \rho_t(x) \right), \tag{59}$$

while the jump part of the local symmetric velocity reads

$$v_t^J(x) = \frac{\int dy W_t(x, y)(y - x) - \rho_t^{-1}(x) \int dy \rho_t(y) W_t(y, x)(y - x)}{2}. \tag{60}$$

Finally, the stochastic symmetric derivative (32) takes the form

$$\frac{d}{dt} = \partial_t + \left(\widehat{u}_t^i - \frac{d_t^{ij}}{2} (\nabla_j \ln \rho_t) \right) \nabla_i + \frac{W_t - \rho_t^{-1} \circ W_t^\dagger \circ \rho_t - \lambda_t \mathscr{I} + \rho_t^{-1} W_t^\dagger [\rho_t] \mathscr{I}}{2}. \tag{61}$$

Here, we are in the general case where the link between equilibrium ($V = 0$) and local symmetric velocity is shown in Fig. 2. However, we remark that the condition

$$\widehat{u}_t = \frac{d_t}{2} (\nabla \ln \rho) \quad \text{and} \quad \rho(x) W_t(x, y) = \rho(y) W_t(y, x) \tag{62}$$

is a sufficient and a necessary condition to be in equilibrium ($V = 0$).[9]

A particular form of such jump diffusion process (52), that we call jump Langevin equation, is obtained from the Langevin equation (44) by adding a Poisson noise w_t, as

$$\dot{x}^i = -\Gamma_t^{ij}(x)\partial_j H_t(x) + G_t^i(x) + \frac{1}{2}\partial_{y^j} D_t^{ij}(x, y)\Big|_{x=y} + \eta_t^i(x) + w_t^i(x), \tag{63}$$

with $d_t^{ij}(x) = \frac{2}{\beta}\Gamma_t^{ij}(x)$ such that the transition rate, (56), takes the particular form (Kangaroo process [8])

$$W_t(x, y) = r \exp\left(-\frac{\beta}{2}\big(H_t(y) - H_t(x)\big)\right), \tag{64}$$

where r is real. The accompanying density (13), in the case without external force ($G_t = 0$), is the Gibbs density $\frac{\exp(-\beta H_t)}{Z_t}$. If, in addition, we have a stationary Hamiltonian ($H_t = H$), such processes verify the sufficient equilibrium condition (62) in this Gibbs density $\rho(x) = \frac{\exp(-\beta H(x))}{Z}$. We will now consider physical examples of jump diffusion process (52).

4.3.1 Example 1: Interlacing Levy Process on the Unit Circle

The most elementary example of an interlacing Levy process which describes a nonequilibrium system is a particle on a unit circle subject to a constant force G, as

$$\dot{\theta}_t = G + \eta_t + w_t, \tag{65}$$

with an additive and stationary Gaussian white noise ($d_t^{ij}(\theta) = d$) and a state-independent and stationary Poisson white noise ($\lambda_t(\theta) = \lambda$ and $b_{t,\theta}(\theta') = b(\theta')$). Moreover, the jump amplitude is a periodic function, $b(\theta) = b(\theta + 2\pi)$. The Fokker-Planck equation (9) becomes, with (55),

$$\partial_t \rho_t(\theta) = -G\partial_\theta \rho_t(\theta) + \frac{d}{2}\partial_{\theta\theta}^2 \rho_t(\theta) - \lambda\rho_t(\theta) + \lambda \int_0^{2\pi} d\theta' b(\theta - \theta')\rho_t(\theta'). \tag{66}$$

Then, the process possesses an invariant probability distribution with the constant density $\rho(\theta) = \frac{1}{2\pi}$. This is true also in the absence of Poisson noise ($\lambda = 0$) or Gaussian noise ($d = 0$). For the stationary process, where we take the invariant density as initial density, the velocity operator (57,58) takes the form

$$V[f](\theta) = 2G\partial_\theta f + \lambda \int_0^{2\pi} d\theta' \big(b(\theta' - \theta) - b(\theta - \theta')\big) f(\theta'). \tag{67}$$

In the absence of external force (i.e., $G = 0$), we see that the Poisson noise transforms an equilibrium state to a nonequilibrium steady state if b is not an even function. Finally, the local symmetric velocity takes the form (57,59,60)

$$v(\theta) = G + \frac{\lambda}{2}\int_0^{2\pi} d\theta'\theta' \big(b\left(\theta' - \theta\right) - b\left(\theta - \theta'\right)\big). \tag{68}$$

[9] That the condition is necessary follows from the fact we can split up the kernel V_t into a regular and a distributional part, and both should vanish to ensure that $V_t = 0$.

For example, if we choose the probability of the jump distribution as $b(\theta) = \frac{1+\sin(\theta)}{2\pi}$, then the local symmetric velocity in the steady state takes the form $v(\theta) = G + \frac{\lambda}{2\pi}\int_0^{2\pi} d\theta' \times \sin(\theta' - \theta)\theta' = G - \lambda\cos(\theta)$. So, despite the fact that the Poisson noise does not change the invariant density, it changes the local symmetric velocity which is no longer constant around the circle. For example, if $G < \lambda$, it includes regions of the circle where the local transport is in the reverse sense to the external force.

4.3.2 Example 2: Jump Langevin Equation on the Unit Circle

We consider a particular case of (63), namely,

$$\dot{\theta}_t = -\partial_\theta H + G + \eta_t + w_t, \tag{69}$$

which describes the angular position of an overdamped particle on a circle. The Hamiltonian H is 2π-periodic, the force G is a constant, the Gaussian white noise η_t has the covariance $\langle \eta_s \eta_t \rangle = \frac{2}{\beta}\delta(t-s)$, and the transition rates of the state-dependent Poisson white noise are given by (64). Such systems without the Poisson noise ($r = 0$) have been realized with a colloidal particle kept by an optical tweezer on a nearly circular orbit [38]. In these experiments, $H(\theta) = a\sin\theta$. In this case, the invariant density takes the form [12]

$$\begin{aligned}\rho(\theta) &= Z^{-1}\exp(-\beta\{H(\theta) - G\theta\}) \\ &\quad \times \left(\int_0^\theta \exp(\beta\{H(\vartheta) - G\vartheta\})d\vartheta + \exp(2\pi\beta G)\int_\theta^{2\pi} \exp(\beta\{H(\vartheta) - G\vartheta\})d\vartheta\right),\end{aligned} \tag{70}$$

where Z is the normalization factor. The corresponding local symmetric velocity (also the hydrodynamic velocity in the present context) takes the form

$$v(\theta) = \beta^{-1}Z^{-1}\frac{\exp(2\pi\beta G) - 1}{\rho(\theta)}. \tag{71}$$

However, with the Poisson noise ($r \neq 0$), it is not possible to obtain analytically the form of the stationary state, except in the equilibrium case (i.e., without external force, $G = 0$), where the equilibrium density is

$$\rho(\theta) = Z^{-1}\exp(-\beta H(\theta)), \tag{72}$$

and the local symmetric velocity is zero. We realize a numerical simulation of the system (69) with $a = 0.87s^{-1}$ and $\beta = 0.8s$ (these values for a and β are close to those used in the experiment [38]), but with a non-vanishing Poisson noise ($r \neq 0$). We can imagine for example that it is once again the laser beam which produces the two noise. We first verify numerically that we find the equilibrium density (72) for three values of $r = 0.001, 0.01$, and 0.1 in the case $G = 0$. The results of the numerical simulation are shown in Fig. 4 which confirm the independence of the equilibrium density on the Poisson noise.

Next, we investigate numerically the case where the external force takes the value of the experiments [38] ($G = 0.85s^{-1}$) for three different values of r (which characterizes the role of the Poisson noise), namely, $r = 0.0001, 0.001$, and 0.1. The corresponding forms of the stationary state distribution are shown in Fig. 5(b). From the figure, it is evident that in the presence of the external force, the form of the non-equilibrium stationary state depends on

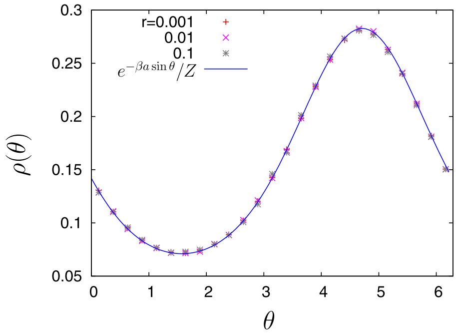


Fig. 4 The points in the figure show the equilibrium density $\rho(\theta)$, obtained from numerical simulations of the dynamics (69) with $H = a\sin\theta$, and with $G = 0$, $a = 0.87s^{-1}$, $\beta = 0.8s$, and for three values of $r = 0.001, 0.01$, and 0.1. It can be seen that the results do not depend on the value of r. In the figure, the results of numerical simulations have also been compared with the analytical result given in (72) with $H = a\sin\theta$, and is represented in the figure by the continuous line

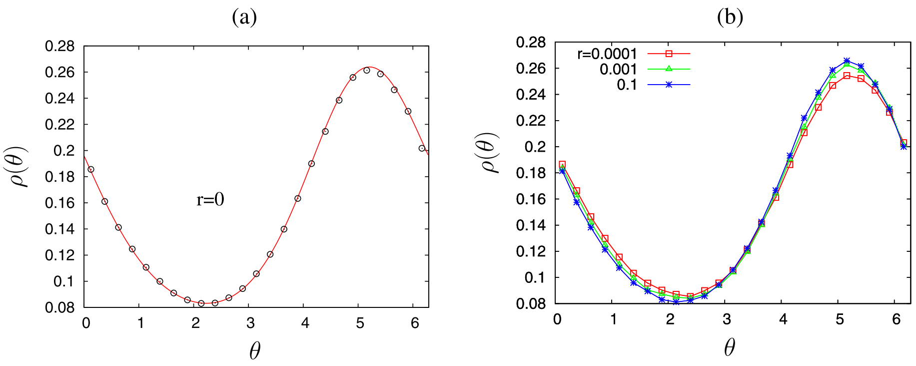


Fig. 5 (**a**) The points represent the stationary density $\rho(\theta)$, obtained from numerical simulation of the dynamics (69) with $H = a\sin\theta$, and with $G = 0.85s^{-1}$, $a = 0.87s^{-1}$, $\beta = 0.8s$, but without the Poisson noise ($r = 0$). As expected, the points may be seen to lie on the continuous line representing the exact result in (70). (**b**) Here, we show the stationary density $\rho(\theta)$, obtained from numerical simulations of the dynamics (69) with $G = 0.85s^{-1}$, $a = 0.87s^{-1}$, $\beta = 0.8s$, and for $r = 0.0001, 0.001$, and 0.1. It is easily seen that $\rho(\theta)$ depends on the value of r, thereby hinting at the important role played by the Poisson noise

r, thereby underlying the importance of the Poisson noise. This is to be contrasted with the result for the case depicted in Fig. 4, i.e., with $G = 0$, when the form of the equilibrium stationary state is independent of r. Corresponding to the non-equilibrium stationary state for $G \neq 0$, the local symmetric velocity (57,59,60) is given by

$$\begin{aligned} v(\theta) &= -a\cos(\theta) + G - \frac{1}{\beta}\partial_\theta\left(\ln\rho(\theta)\right) \\ &\quad + \frac{r\exp(\frac{a\beta}{2}\sin(\theta))}{2}\left(\int_0^{2\pi} d\theta' \exp\left(-\frac{\beta a}{2}\sin(\theta')\right)\theta'\right) \\ &\quad - \frac{r\rho^{-1}(\theta)\exp(-\frac{a\beta}{2}\sin(\theta))}{2}\left(\int_0^{2\pi} d\theta' \rho(\theta')\exp\left(\frac{\beta a}{2}\sin(\theta')\right)\theta'\right). \end{aligned} \tag{73}$$

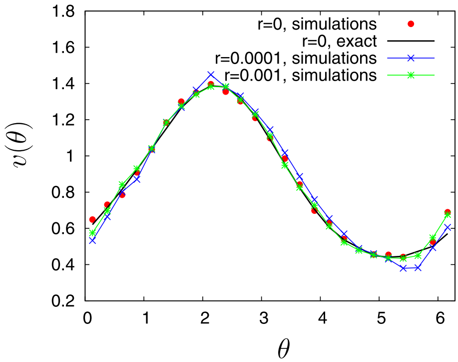


Fig. 6 The figure shows the local symmetric velocity $v(\theta)$ for the dynamics (69) with $H = a \sin\theta$, and with $G = 0.85 s^{-1}$, $a = 0.87 s^{-1}$, $\beta = 0.8 s$, and for $r = 0$ (no Poisson noise), 0.0001, and 0.001. The points are obtained from numerical simulations of the dynamics and use of the formula (73). The exact result for the case $r = 0$ is given by (71). It is easily seen that $v(\theta)$ depends on the value of r, i.e., on the details of the Poisson noise in the dynamics

In Fig. 6, we show the local symmetric velocity $v(\theta)$ for the dynamics (69) with $G = 0.85 s^{-1}$, $a = 0.87 s^{-1}$, $\beta = 0.8 s$, and for $r = 0$ (no Poisson noise), 0.0001, and 0.001. It is clear from the figure that the quantity $v(\theta)$ depends on the details of the Poisson noise in the dynamics.

In Sect. 5.3.1, we will use the dynamics (69) as a model system to verify the **GFDT** by extensive numerical simulations.

5 Perturbation of a Markov Process: The Fluctuation-Dissipation Theorem

Suppose that our dynamics evolves for $t \leq 0$ with a given Markovian dynamics of generator L_t and then suddenly, at time $t = 0$, we perturb the dynamics such that the new Markov generator L'_t becomes

$$L'_t = L_t + k_t N_t, \tag{74}$$

with k_t a real function, sometimes called the response field, and N_t an operator. We will assume that the perturbed process still has the property to have honest transition probability (i.e., $N_t[1] = 0$). The **FDT** concerns the relation between correlation functions, (34), in the unperturbed state and response functions in the case of a small perturbation (i.e., k_t infinitesimal).

5.1 Response Function

The linear response theory allows to express the variation of the average of an observable under the perturbation as

$$\left.\frac{\delta \langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \left\langle \left(\rho_s^{-1} N^{\dagger}[\rho_s]\right)(x_s) A_t(x_t) \right\rangle, \tag{75}$$

where $\langle\rangle'$ denotes expectation for the process with the generator L'_t. The proof of this relation is given in Appendix C for the convenience of the reader. Note however that this result is known for a long time in the physics literature [1, 41, 53, 80] and now has a mathematically rigorous formulation (Definition 2.5 in [25]). This relation, besides being the basis for the **FDT**, allows to prove the Green-Kubo relation [54] in the case of homogeneous perturbation ($k_t = k$) of a stationary dynamics. Note that other higher order relations may be derived in the context of the non-linear response theory [61].

5.2 Hamiltonian Perturbation Class or Generalized Doob h-Transform

We will see that the form of the perturbation is the central point of the **FDT**, and it does not make sense to talk of **FDT** without giving its form. We want to begin by studying a class of (non-infinitesimal) perturbation of the Markov process such that the transformation of the generator can be expressed in terms of a family of non-homogeneous positive function h_t, as

$$L_t' = h_t^{-1} \circ L_t \circ h_t - h_t^{-1} L_t[h_t] \equiv L_t^h. \tag{76}$$

In the case where $\frac{d_+ h_t}{dt} = \partial_t h_t + L_t[h_t] = 0$ ($h_t(x)$ is the so-called space time harmonic function), such a transformation is classical in the probability literature and is called the Doob h-transform (or gauge transformation in physics literature). This was first introduced by Doob ([28]; see also Chap. 11 of [16]), and plays an important role in the potential theory. We remark that if $h_t(x)$ is space-time harmonic, then $h_t(x_t)$ is a **martingale**, i.e.,

$$h_t(x) = \mathbf{E}_{t,x}\left(h_T(x_T)\right) \quad \forall T \geq t. \tag{77}$$

By introducing the symmetric bilinear operator Γ (the so-called "carre du champs" [79], which can be roughly translated into English as "square of the field"), such that $\Gamma_t(f, g) = L_t[fg] - f L_t[g] - L_t[f]g$, the perturbed generator can be expressed in the form $L_t^h = L_t + h_t^{-1}\Gamma(h_t,)$. A remarkable property of this type of perturbation appears if we restrict to a subclass of unperturbed processes which are in so-called local detailed balance (14) with the Gibbs density $\pi_t = \exp(-\beta H_t)$. We then have the relation

$$\begin{aligned} h_t^2\pi_t \circ L_t^h \circ \left(h_t^2\pi_t\right)^{-1} &= h_t\pi_t \circ L_t \circ (\pi_t)^{-1} h_t^{-1} - h_t^{-1} L_t(h_t) \\ &= h_t \circ L_t^\dagger \circ h_t^{-1} - h_t^{-1} L_t(h_t) = \left(L_t^h\right)^\dagger, \end{aligned} \tag{78}$$

which implies that, for the perturbed process, the density, given by

$$\pi_t^h = \pi_t h_t^2 = \exp(-\beta H_t + 2\ln h_t), \tag{79}$$

is also in local detailed balance. This property of conservation of instantaneous infinitesimal detailed balance under the perturbation of the Hamiltonian $H \to H - \frac{2}{\beta}\ln h_t$ is the first justification for the name "Hamiltonian perturbation" that we chose for this type of perturbation. However, we stress that this perturbation, although called here "Hamiltonian perturbation", is applicable to general Markov processes which do not have an underlying Hamiltonian which generates the dynamics. Moreover, for a general diffusion process, we can easily calculate (see Appendix D) the operator "carre du champs"

$$\Gamma_t(f, g) = d_t^{ij}(\nabla_i f)(\nabla_j g). \tag{80}$$

Then the perturbed generator (76) is

$$L_t^h = L_t + d_t^{ij}\nabla_j\left(\ln|h_t|\right)\nabla_i, \tag{81}$$

so that there is just a change of the drift term, $u_t^i \to u_t^i + d_t^{ij}\nabla_j(\ln h_t)$. In the subcase of an overdamped Langevin process (44), the perturbed process (76) becomes

$$\dot{x}^i = -\Gamma_t^{ij}(x)\partial_j\left(H_t(x) - \frac{2}{\beta}\ln h_t\right) + G_t^i(x) + \frac{\partial_{y^j} D_t^{ij}(x,y)|_{x=y}}{2} + \eta_t^i(x). \tag{82}$$

So we see that the perturbation in (76) is once again equivalent to change of the Hamiltonian, $H \to H - \frac{2}{\beta}\ln h_t$. Now we want to show that the type of perturbation in (76) includes the perturbation usually considered in the articles on **FDT** that exist in the literature.

– For pure jump process, it is usual to ask precisely the property of conservation of this local detailed balance for the Gibbs density $\pi_t = \exp(-\beta H_t)$ under the perturbation of the Hamiltonian $H \to H - k_t O_t$. We see from (79) that this perturbation of the Hamiltonian is of the type in (76), with the choice

$$h_t = \exp\left(\frac{\beta}{2}k_t O_t\right). \tag{83}$$

  This implies the following transformation for the transition rates.

$$W_t^h(x,y) = \exp\left(-\frac{\beta}{2}k_t O_t(x)\right)W_t(x,y)\exp\left(\frac{\beta}{2}k_t O_t(y)\right). \tag{84}$$

  This is the perturbation considered recently in [3] and earlier in [27] for finding the **GFDT** in this pure jump process set-up.
– For overdamped Langevin process, it is usual [41, 53, 68, 80] to do a perturbation of the Hamiltonian, $H \to H - k_t O_t$, in (44). With (82), we see that it is of the type in (76) with once again (83) valid.
– Finally, we remark that for a jump diffusion process of type (52), this perturbation consists of a change of the drift according to $u_t^i \to u_t^i + d_t^{ij}\nabla_j(\ln h_t)$ and simultaneously, a perturbation of the jump process by replacing the transition rates (56) by

$$W_t^h(x,y) = h_t^{-1}(x)W_t(x,y)h_t(y).$$

  For the jump Langevin process (63), with the transition rates (64) for the Poisson noise, we can prove easily that the choice (83) in (76) is equivalent to the perturbation of the Hamiltonian according to $H \to H - k_t O_t$.

5.3 Fluctuation-Dissipation Theorem for Hamiltonian Perturbation

In the case of an infinitesimal h_t function,

$$h_t(x) = 1 + k_t B_t(x) + O(k^2), \tag{85}$$

we find that the Hamiltonian perturbation (76) has the infinitesimal form (74) with

$$N_t = L_t \circ B_t - B_t \circ L_t - L_t[B_t]\mathscr{I}. \tag{86}$$

The central point of the proof that follows is the fact that the observable $\rho^{-1}N_t^{\dagger}[\rho]$, which appears on the right hand side of (75), can be expressed in terms of the stochastic derivative (associated with the unperturbed process) of the observable B_t.

$$\rho_t^{-1}N_t^{\dagger}[\rho_t] = B_t\rho_t^{-1}L^{\dagger}[\rho_t] - \rho_t^{-1}\circ L^{\dagger}\circ\rho_t[B_t] - L_t[B_t]$$

$$= -(L_t + L_t^*)[B_t] = \left(\frac{d_-}{dt} - \frac{d_+}{dt}\right)[B_t], \tag{87}$$

where the third equality comes from (30). We can rewrite this observable by adding a term proportional to $(2\frac{d}{dt} - \frac{d_-}{dt} - \frac{d_+}{dt})B$ (which is exactly equal to zero), and then, for all α, we get

$$\rho_t^{-1} N_t^\dagger[\rho_t] = (1-\alpha)\frac{d_-}{dt} B_t - (1+\alpha)\frac{d_+}{dt} B_t + 2\alpha \frac{d}{dt} B_t. \tag{88}$$

Now, by using the response relation, (75) and the time derivative of a correlation function, (35), we find the family, indexed by α, of equivalent **GFDT**.

$$\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0}$$
$$= (1-\alpha)\,\partial_s\,\langle B_s(x_s)A_t(x_t)\rangle - (1+\alpha)\left\langle \frac{d_+ B_s}{ds}(x_s)A_t(x_t)\right\rangle + 2\alpha\left\langle\frac{dB_s}{ds}(x_s)A_t(x_t)\right\rangle. \tag{89}$$

Two particular cases of α exist in the literature:

– $\alpha = 0$: **First GFDT**

$$\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s\,\langle B_s(x_s)A_t(x_t)\rangle - \left\langle\frac{d_+ B_s}{ds}(x_s)A_t(x_t)\right\rangle \tag{90}$$

$$= \partial_s\,\langle B_s(x_s)A_t(x_t)\rangle - \langle(\partial_s B_s)\,(x_s)A_t(x_t)\rangle - \langle(LB)_s\,(x_s)A_t(x_t)\rangle\,. \tag{91}$$

In the usual case of Hamiltonian perturbation of a jump process or an overdamped Langevin process, with (83), we find $B_t = \frac{\beta}{2} O_t$ and then

$$\frac{2}{\beta}\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s\,\langle O_s(x_s)A_t(x_t)\rangle - \left\langle\frac{d_+ O_s}{ds}(x_s)A_t(x_t)\right\rangle \tag{92}$$

$$= \partial_s\,\langle O_s(x_s)A_t(x_t)\rangle - \langle(\partial_s O_s)\,(x_s)A_t(x_t)\rangle - \langle(LO)_s\,(x_s)A_t(x_t)\rangle\,, \tag{93}$$

which was first written down in [20] for diffusion process with additive noise and recently in [3, 4, 60, 64, 83] for jump process and overdamped Langevin process. The equilibrium limit (1) is a bit obscure; it may be seen by noting that one has $\langle(LO)(x_s)A(x_t)\rangle = \langle A(x_s)(LO)(x_t)\rangle = \partial_t\langle A(x_s)O(x_t)\rangle$. However, there exists physical interpretation of the new term $\langle(LB)_s(x_s)A_t(x_t)\rangle$ as the "frenetic term" [3, 4].

– $\alpha = -1$: **Second GFDT**

$$\frac{1}{2}\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s\,\langle B_s(x_s)A_t(x_t)\rangle - \left\langle\frac{dB_s}{ds}(x_s)A_t(x_t)\right\rangle, \tag{94}$$

which has the advantage that the effect of the nonequilibrium character of the unperturbed state is just in the second term on the right hand side. For a diffusion process, this **GFDT** can be written [12–14], with (49), as

$$\frac{1}{2}\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s\,\langle B_s(x_s)A_t(x_t)\rangle - \langle(\partial_s B_s)\,(x_s)A_t(x_t)\rangle - \left\langle\left(V_s^c.\nabla B_s\right)(x_s)A_t(x_t)\right\rangle. \tag{95}$$

This **GFDT** was experimentally checked in [38]. In the usual case of Hamiltonian perturbation of a pure jump process or a overdamped Langevin process, with (83), we find

$$\frac{1}{\beta}\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\bigg|_{k=0} = \partial_s\,\langle O_s(x_s)A_t(x_t)\rangle - \left\langle \frac{dO_s}{ds}(x_s)A_t(x_t)\right\rangle. \tag{96}$$

5.3.1 Example of Jump Langevin Equation (4.3.2)

Here, we want to numerically verify the **GFDT** (94) for a Markov process which mixes jump and diffusion. We consider the stochastic dynamics (69) with $H = a\sin\theta$ and the same values for the parameters as those considered in (4.3.2); $a = 0.87s^{-1}$, $G = 0.85s^{-1}$, $\beta = 0.8s$, and $r = 0.001$. The process is supposed to be at time $t \le 0$ in the stationary state with $\rho(\theta)$ given in Fig. 5(b). Then, suddenly, at $t = 0$, we consider a static perturbation of the Hamiltonian according to

$$H' = H - k\sin\theta = (a-k)\sin\theta. \tag{97}$$

We saw in the last section that this perturbation is of the form (76), with

$$h(\theta) = \exp\left(\frac{\beta}{2}k\sin\theta\right). \tag{98}$$

We checked numerically the time integrated version of the **FDT** (96) around steady state for $A = B = \sin\theta$.

$$\frac{1}{\beta}\frac{\partial}{\partial k}\,\langle \sin\theta_t\rangle'\,\big|_{k=0} = \left\langle \sin^2\theta_t\right\rangle - \langle \sin\theta_0\sin\theta_t\rangle - \int_0^t ds\,\langle C(\theta_s)\sin\theta_t\rangle\,. \tag{99}$$

The form of the observable $C(\theta) \equiv \frac{d\sin\theta_t}{dt}(\theta)$ is found with the help of (61) as

$$\begin{aligned} C(\theta) = &\left(-a\cos(\theta) + G - \frac{1}{\beta}(\partial_\theta \ln\rho)\right)\cos\theta \\ &+ \frac{(\int d\theta' W(\theta,\theta')(\sin(\theta') - \sin(\theta)))}{2} \\ &- \frac{\rho^{-1}(\theta)(\int d\theta'(\sin(\theta') - \sin(\theta))\rho(\theta')W(\theta',\theta))}{2}, \end{aligned} \tag{100}$$

with $W(\theta,\theta')$ given by (64)

$$W(\theta,\theta') = r\exp\left(-\frac{\beta a}{2}\left(\sin(\theta') - \sin(\theta)\right)\right). \tag{101}$$

Figure 7 shows results from our numerical simulations for the various terms in the integrated version of the **GFDT** (99). In the figure, one can observe a satisfactory agreement between the left hand side and the right side of (99), thereby verifying the **GFDT**.

5.4 Fluctuation-Dissipation Theorem for a More General Class of Perturbation

We will now consider a larger class of perturbation than (76) such the perturbation can be expressed in terms of two family of non-homogeneous functions h_t and h'_t, as

$$L'_t = h_t^{-1}\circ L_t \circ h'_t - h_t^{-1}\circ L_t[h'_t], \tag{102}$$

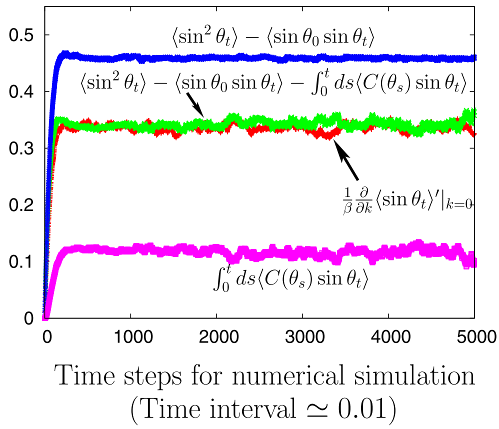


Fig. 7 Based on our results from numerical simulations of the dynamics (69) with $H = a\sin\theta$, the figure shows the different terms in the integrated version of the **GFDT** (99). Here, $a = 0.87s^{-1}$, $G = 0.85s^{-1}$, $\beta = 0.8s$, and the parameter $r = 0.001$. One observes a satisfactory agreement between the left hand side $\frac{1}{\beta}\frac{\partial}{\partial k}\langle\sin\theta_t\rangle'|_{k=0}$ and the right side $\langle\sin^2\theta_t\rangle - \langle\sin\theta_0\sin\theta_t\rangle - \int_0^t ds\langle C(\theta_s)\sin\theta_t\rangle$ of the **GFDT** (99), which therefore verifies the theorem

which specializes to the Hamiltonian perturbation (76) when $h = h'$. We will see in the following subsections two physical perturbations, the time change and the thermal perturbation, which belong to this class. In the case of infinitesimal perturbation,

$$h_t = 1 + k_t B_t + O(h^2) \quad \text{and} \quad h'_t = 1 + k_t B'_t + O(h^2), \tag{103}$$

we find that this perturbation has the form (74) with

$$N_t = -B_t \circ L_t + L_t \circ B'_t - L_t[B'_t]. \tag{104}$$

For a pure discontinuous process, the perturbation (102) implies for the transition rates, $W'_t = h_t^{-1} \circ W_t \circ h'_t$, and was considered in [27] and more recently in [67] by taking $h_t(x) = \exp(\mu\beta k_t O(x))$ and $h'_t(x) = \exp(\gamma\beta k_t O(x))$, where $O(x)$ is an observable, and μ and γ two real numbers. As in (87), we show that the observable $\rho_t^{-1}N_t^\dagger[\rho_t]$, which appears on the right hand side of (75), can be expressed in terms of the stochastic derivative of B_t and B'_t as

$$\begin{aligned}\rho^{-1}N^+[\rho] &= -\rho^{-1}\circ L^\dagger \circ \rho[B] + B'\rho^{-1}L^\dagger[\rho] - L[B'] \\ &= -L^*[B] - B\rho^{-1}L^\dagger[\rho] + B'\rho^{-1}L^\dagger[\rho] - L[B'] \\ &= \begin{cases} (\partial_t + \rho^{-1}L^\dagger[\rho])(-B+B') + \frac{d_- B}{dt} - \frac{d_+ B'}{dt} \\ \text{or, } (\partial_t + \rho^{-1}L^\dagger[\rho])(-B+B') + \frac{d_-(B'+B)}{dt} - 2\frac{dB'}{dt}. \end{cases}\end{aligned}$$

We obtain then the generalization of the first **GFDT** (91)

$$\begin{aligned}&\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} \\ &= \partial_s\langle B_s(x_s)A_t(x_t)\rangle - \left\langle \frac{d_+B'_s}{ds}(x_s)A_t(x_t)\right\rangle \\ &\quad + \left\langle\left(\left(\partial_s + \rho_s^{-1}L_s^\dagger[\rho_s]\right)(B'_s - B_s)\right)(x_s)A_t(x_t)\right\rangle,\end{aligned} \tag{105}$$

and the second **GFDT** (94)

$$\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0}$$

$$= \partial_s \left\langle \left(B'_s + B_s\right)(x_s)A_t(x_t)\right\rangle - 2\left\langle \frac{dB'_s}{ds}(x_s)A_t(x_t)\right\rangle$$

$$+ \left\langle \left(\left(\partial_s + \rho_s^{-1}L_s^{\dagger}[\rho_s]\right)(B'_s - B_s)\right)(x_s)A_t(x_t)\right\rangle. \quad (106)$$

We see that in the Hamiltonian perturbation class (i.e., $B = B'$), we recover the **GFDT** (91,94).

5.4.1 *Around Steady State*

We will now restrict to the case where the observable does not have explicit time dependence (i.e., $A_t = A$, $B_t = B$, $B'_t = B'$), and the unperturbed state is a steady state. Then the first **GFDT** (105) becomes

$$\left.\frac{\delta\langle A(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s \langle B(x_s)A(x_t)\rangle - \left\langle \frac{d_+B'}{ds}(x_s)A(x_t)\right\rangle, \quad (107)$$

and the second (106) becomes

$$\left.\frac{\delta\langle A(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s \left\langle \left(B + B'\right)(x_s)A(x_t)\right\rangle - 2\left\langle \frac{dB'}{ds}(x_s)A(x_t)\right\rangle. \quad (108)$$

In the case where the steady state is of equilibrium-type (i.e. $\frac{d}{ds} = \partial_s$), this last relation (108) simplifies to the form

$$\left.\frac{\delta\langle A(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s \left\langle \left(B + B'\right)(x_s)A(x_t)\right\rangle. \quad (109)$$

5.4.2 *Time Change for a Homogeneous Markov Process* [25]

An example of perturbation which belongs to the generalized class (102) but not to the Hamiltonian perturbation class (76) is when we consider the change of clock as follows.

$$t^f(s) \equiv \int_0^s du \exp\left(f_u(x_u)\right), \quad (110)$$

where f_u is an observable. It is proved in [25] (Proposition 3.1) that the process $x'_s = x_{t^f(s)}$ is still Markov with a generator $L'_t = \exp(-f_t)L$. In the case of infinitesimal perturbation $f_u(x) = k_u B(x)$, $L'_t = L - k_t BL$, which is of the form (104) with $B' = 0$ so that the FDT (105, 106) takes the form

$$\left.\frac{\delta\langle A(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s \langle B(x_s)A(x_t)\rangle - \left\langle \left(\rho_s^{-1}L^{\dagger}[\rho_s]B\right)(x_s)A(x_t)\right\rangle. \quad (111)$$

In the case of an unperturbed system in the steady state, (107,108) become the usual **FDT**.

$$\left.\frac{\delta\langle A(x_t)\rangle'}{\delta k_s}\right|_{k=0} = \partial_s \langle B(x_s)A(x_t)\rangle, \quad (112)$$

which is a result of [25]. We want to emphasize that, for this type of perturbation, we obtain the usual **FDT** (without correction) for an unperturbed state which is a general nonequilibrium steady state.

5.4.3 Thermal Perturbation Pulse: Change of Temperature for Equilibrium Overdamped Langevin Process

A famous example in physics for a perturbation which is not of Hamiltonian type is thermal perturbation. Let us consider a system whose dynamics is governed by (44), with $G = 0$ and homogeneous Hamiltonian, and the perturbed system which results from the change of the bath temperature $\beta_t^{-1} = (1 + k_t)\beta^{-1}$. We can easily prove that

$$N = \frac{1}{\beta}\nabla_i \circ \Gamma^{ij} \circ \nabla_j, \tag{113}$$

which is of the form of the general infinitesimal perturbation (104) with $B' = \frac{\beta H}{2}$ and $B = \frac{\beta H}{2} - 1$. This can be easily seen by using the formula (80) for the "carre du champs":

$$L \circ B' - L[B'] = B'L + \Gamma(B', .) = B'L + \frac{2\Gamma^{ij}}{\beta}\left(\nabla_i B'\right)\nabla_j = \frac{\beta H}{2} L - L + N. \tag{114}$$

The formula (109) then takes the form $\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}|_{k=0} = \partial_s\langle(\beta H - 1)(x_s)A_t(x_t)\rangle$, which implies the equilibrium form

$$\frac{1}{\beta}\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\bigg|_{h=0} = \partial_s\left\langle H(x_s)A_t(x_t)\right\rangle. \tag{115}$$

In particular, we obtain the usual **FDT** for the energy [80].

$$\frac{1}{\beta}\frac{\delta\langle H(x_t)\rangle'}{\delta k_s}\bigg|_{k=0} = \partial_s\left\langle H(x_s)H(x_t)\right\rangle. \tag{116}$$

6 Two Families of Non-perturbative Extensions of the Fluctuation-Dissipation Theorem

It is well understood since the discovery of the **FR** that they may be viewed as extensions to the non-perturbative regime of the Green-Kubo and Onsager relations which are usually valid within the linear response description in the vicinity of equilibrium [36, 59]. A detailed proof was given in [11] that the Jarzynski equality gives the usual **FDT** when expanded to second order in the response field. In [12], it was proved that this correspondence is still true around an unperturbed state which is stationary but out of equilibrium). This is proved by doing a Taylor expansion of a special Crooks theorem to first order in the response field. Finally, in [14], general **FR** were exhibited which are global versions of the **GFDT** for nonequilibrium diffusion, or, of the **FDT** for energy resulting from a thermal perturbation. We introduce in Sect. 6.1 a first family of exponential martingales which is a natural object associated with the perturbation (76), and show in Sect. 6.1.3 that these are global version of general **GFDT** (91,94). Section 6.2 presents the martingale property of functionals which appear in the fluctuation relations and it shows their relation to the exponential martingales introduced in Sect. 6.1. Along the way, we prove the **FR** along the lines of the proof given below for the exponential martingale by a comparison to the backward process generated by the Doob h-transform of the adjoint generator $L^\dagger$.

6.1 New Family of Exponential Martingales Naturally Related to **GFDT**

6.1.1 Introduction

We come back to the perturbation (76) of the generator,

$$L_t^h \equiv h_t^{-1} \circ L_t \circ h_t - h_t^{-1} L_t[h_t], \tag{117}$$

but this time we will not restrict to the regime where h_t is infinitesimal. We prove in Appendix E that the Markov process associated with the generators L_t^h and L_t are related through the functional $\exp(-\mathbf{Z}_s^{h,t})$ by

$$P_s^{h,t}(x,y) = \mathbf{E}_{s,x}\left[\delta(x_t - y)\exp(-\mathbf{Z}_s^{h,t})\right], \tag{118}$$

where

$$\exp(-\mathbf{Z}_s^{h,t}[x]) = h_s^{-1}(x_s)\exp\left(-\int_s^t du\left(h_u^{-1}L_u[h_u] + h_u^{-1}\partial_u h_u\right)(x_u)\right)h_t(x_t). \tag{119}$$

The functional $\exp(-\mathbf{Z}_s^{h,t})$ is multiplicative:

$$\exp(-\mathbf{Z}_s^{h,t}) = \exp(-\mathbf{Z}_s^{h,u})\exp(-\mathbf{Z}_u^{h,t}) \tag{120}$$

for $s \le u \le t$. The perturbation (117) is a particular case of the transformation of a Markov process by multiplicative functionals [7, 45]. It is a generalization of the Doob h-transform, which is

$$P_s^{h,t}(x,y) = h_s^{-1}(x)P_s^t(x,y)h_t(y), \tag{121}$$

in the case where $h_t(x)$ is the space-time harmonic function, i.e. $\frac{d_+h}{dt} = 0$.

Thanks to the Markovian structure of the trajectory measure, the relation (118) for the transition probability is equivalent (as proved in Appendix F) to the relation between the expectations of functionals of the paths from time s to time t for the perturbed and the unperturbed processes,

$$\mathbf{E}_{s,x}^h\left[F_{[s,t]}\right] = \mathbf{E}_{s,x}\left[F_{[s,t]}\exp(-\mathbf{Z}_s^{h,t}[x])\right], \tag{122}$$

where $\mathbf{E}_{s,x}^h[\ ]$ denotes expectation for the process with generators L_t^h.

Finally, we can also formulate (122) by requiring that the perturbed process with generators L_t^h and trajectory measure $M_{\mu_{0,[s,t]}}^h$,[10] can be obtained from the unperturbed process with trajectory measure $M_{\mu_{0,[s,t]}}$ by using the likelihood ratio process (the Radon-Nikodym density):

$$M_{\mu_{0,[s,t]}}^h[x] = M_{\mu_{0,[s,t]}}[x]\frac{\rho_s^h}{\rho_s}(x_s)\exp(-\mathbf{Z}_s^{h,t}[x]), \tag{123}$$

with $\rho_s(x) = \int dy \rho_0(y)P_0^s(y,x)$ the instantaneous density of the original process and $\rho_s^h(x) = \int dy \rho_0(y)P_0^{h,s}(y,x)$ the instantaneous density of the h-transformed process.

[10]Note that the measure $\mu_0(dx) = \rho_0(x)dx$ is the measure at initial time $t = 0$ and not at time s.

We could not find the general result (119,122,123) in the mathematics literature, but many very closely related results do exist. The subcase of (122,123) where h_t is time-homogeneous (i.e., $\partial_t h_t = 0$)) was treated long time ago by Kunita in [56] and was revisited recently in the articles [76] and [26]. In our context of the **FDT**, the extension to $\partial_t h_t \neq 0$ is essential. But more than generalizing to $\partial_t h_t \neq 0$, the main interest in the Appendices E, F is to prove (122) from theoretical physics perspective. We recall also that for a diffusion process, the perturbed generator (117) is obtained by adding the term $d_t \nabla(\ln h_t(x))$ to the drift (see (81)). Then, the proofs in Appendices E, F are also a theoretical physicist's proofs of the Girsanov theorem for a diffusion process [79] (for this type of change of drift).

6.1.2 *Martingale Properties of the Functional* $\exp(-\mathbf{Z}_s^t)$

The multiplicative functional $\exp(-\mathbf{Z}_s^{h,t}[x])$ is an **exponential martingale** with respect to the natural σ-algebra filtration $\mathscr{F}_t = \sigma(x_s, s \leq t)$ representing the increasing flow of information. This fact can be seen by first noting that (122) (with $F = 1$) implies the normalization condition

$$\mathbf{E}_{s,x}\left[\exp(-\mathbf{Z}_s^{h,t}[x])\right] = 1, \tag{124}$$

which, thanks to the multiplicative structure of $\exp(-\mathbf{Z}_s^{h,t}[x])$, yields

$$\mathbf{E}\left[\exp(-\mathbf{Z}_s^{h,t}[x])|\mathcal{F}_u\right] = \exp(-\mathbf{Z}_s^{h,u}[x])\mathbf{E}_{x_u,u}\left[\exp(-\mathbf{Z}_u^{h,t}[x])\right] = \exp(-\mathbf{Z}_s^{h,u}[x]), \tag{125}$$

for $s \leq u \leq t$.

6.1.3 *Fluctuation-Dissipation Theorem as Taylor Expansion of the Exponential Martingale Identity (122)*

In the infinitesimal case, $h_t(x) = 1 + k_t B_t(x) + O(k^2)$, Taylor expansion of the subcase of (122) with one-point functional $F_{[s,t]}[x] = A_t(x_t)$, namely,

$$\langle A_t(x_t)\rangle^h = \left\langle (h_s)^{-1}(x_s)\exp\left(\int_s^t du\left(-h_u^{-1}L_u[h_u] - h_u^{-1}\partial_u h_u\right)(x_u)\right)h_t(x_t)A_t(x_t)\right\rangle, \tag{126}$$

gives, to the first order in $[k]$,

$$\begin{aligned}&\langle A_t(x_t)\rangle^h - \langle A_t(x_t)\rangle - \left\langle (h_s)^{-1}(x_s)A_t(x_t)\right\rangle - \langle (h_t)(x_t)A_t(x_t)\rangle \\ &\quad + \int_s^t du\left\langle \frac{d_+ h_u}{du}(x_u)A_t(x_t)\right\rangle + O(k^2) = 0.\end{aligned} \tag{127}$$

To find the first **GFDT** (91) from (127), we use the direct differentiation formula $\frac{d_+ h_u}{du} = \frac{d_+(k_u B_u)}{du} = (\partial_u k_u)B_u + k_u\frac{d_+(B_u)}{du}$ obtaining the relation

$$\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_u}\right|_{k=0} - \partial_u\left\langle B_u(x_u)A_t(x_t)\right\rangle + \left\langle \frac{d_+ B_u}{du}(x_u)A_t(x_t)\right\rangle = 0, \tag{128}$$

which is the **GFDT** (91) (note the equivalence of the two notations $\langle\,\rangle'$ and $\langle\,\rangle^h$)). To find the second **GFDT** (94) from (127), we use the formula $d_+ = 2d - d_-$, which gives

$$\langle A_t(x_t)\rangle^h - \langle A_t(x_t)\rangle - \left\langle (h_s)^{-1}(x_s)A_t(x_t)\right\rangle - \langle (h_t)(x_t)A_t(x_t)\rangle$$
$$+2\int_s^t du\left\langle \frac{dh_u}{du}(x_u)A_t(x_t)\right\rangle - \int_s^t du\left\langle \frac{d\_h_u}{du}(x_u)A_t(x_t)\right\rangle + O(k^2) = 0. \quad (129)$$

Then, by using (35) for the time derivative of a correlation function, we obtain

$$\langle A_t(x_t)\rangle^h - \langle A_t(x_t)\rangle - \left\langle (h_s)^{-1}(x_s)A_t(x_t)\right\rangle - \langle (h_t)(x_t)A_t(x_t)\rangle$$
$$+2\int_s^t du\left\langle \frac{dh_u}{du}(x_u)A_t(x_t)\right\rangle - \int_s^t du\,\partial_u\langle h_u(x_u)A_t(x_t)\rangle + O(k^2) = 0. \quad (130)$$

Next, we use the differentiation formula $\frac{dh_u}{du} = \frac{d(k_u B_u)}{du} = (\partial_u k_u)B_u + k_u\frac{d(B_u)}{du}$ to get

$$\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_u}\right|_{k=0} - 2\partial_u\langle B_u(x_u)A_t(x_t)\rangle + 2\left\langle \frac{dB_u}{du}(x_u)A_t(x_t)\right\rangle = 0, \quad (131)$$

which is (94). This gives a second independent proof of (91, 94). It also shows that the above exponential martingales are natural global versions of the **GFDT**. We will discuss in the next section another well known global version, namely, the Fluctuation Relations (**FR**).

6.2 Family of Exponential Martingales Related to **GFDT** Through Fluctuation Relations

6.2.1 Introduction to Fluctuation Relations

Roughly speaking, **FR** may be obtained by comparing the expectation of functionals of trajectories of the system and of reversed trajectories of the so-called backward system[11] (denoted by an index r). More precisely, let us denote by $M^r_{\mu^r_0,[0,T]}$ the trajectorial measure of the backward process which is initially distributed with the measure $\mu^r_0(dx) \equiv \rho^r_0(x)dx$. Next, we define the path-wise time inversion R at fixed time T,[12] which acts on the space of trajectories according to $R[x]_t = [x]_{T-t}$.[13] This allows us to introduce the (push-forward) measure $R_*(M_{\mu_0,[0,T]})$, which is the measure of the trajectory but traversed in the backward sense. We then introduce the action functional $\mathbf{W}_0^T$ through the Radon Nykodym derivative of the image measure of the backward system $R_*(M^r_{\mu^r_0,[0,T]})$ with respect to the trajectorial measure $M_{\mu_0,[0,T]}$ of the forward system (initially distributed with the measure $\mu_0(dx) \equiv \rho_0(x)dx$):[14]

$$R_*\big(M^r_{\mu^r_0,[0,T]}\big) \equiv \exp\big(-\mathbf{W}_0^T\big)M_{\mu_0,[0,T]}. \quad (132)$$

Equivalently, we can write this relation in the form of the Crooks theorem [11, 19, 42, 59, 62, 66, 83] asserting that for all trajectory functionals $F_{[0,T]}$,

$$\big\langle F_{[0,T]}\circ R\big\rangle^r = \big\langle F_{[0,T]}\exp\big(-\mathbf{W}_0^T\big)\big\rangle. \quad (133)$$

[11] It is important to underline that this backward process is not unique. We can also call it a comparison process.

[12] This was also studied in the probabilistic literature, but with time T that could be random [16].

[13] For simplicity, we neglect the case where the time inversion acts non-trivially on the space by an involution. Such a situation arises for Hamiltonian systems (see [11]) where the involution is $(q,p)\to(q,-p)$.

[14] We assume that the measures $M_{\mu_0,[0,T]}$ and $R_*(M^r_{\mu^r_0,[0,T]})$ are mutually absolutely continuous.

Finally, by the substitution $F_{[0,T]}[x] \to F_{[0,T]}[x]\delta(x_0 - y)\delta(x_T - x)$, we find the equivalent relation,

$$\rho_0^r(x)\mathbf{E}_{0,x}^r\left[F_{[0,T]} \circ R[x]\delta(x_T - y)\right] \tag{134}$$

$$= \rho_0(y)\mathbf{E}_{0,y}\left[F_{[0,T]}[x]\exp\left(-\mathbf{W}_0^T[x]\right)\delta(x_T - x)\right]. \tag{135}$$

Due to the freedom in choosing the initial forward measure μ_0 or the backward measure μ_0^r, it is possible to identify the action functional with various thermodynamic quantities like the work performed on the system or the fluctuating entropy creation $\sigma_0^T[x]$ with respect to the inversion r. This latter quantity is obtained when $\mu_0^r(dx) = \rho_0^r(x)dx = \rho_T(x)dx \equiv \int dy\rho_0(y)P_0^T(y,x)dx$. We can also obtain the functional entropy production in the environment, $\mathbf{J}_0^T$, by choosing $\mu_0(dx) = \mu_0^r(dx) = dx$, because then the difference from the entropy creation is the boundary term $\ln(\rho_0(x_0)) - \ln(\rho_t(x_t))$, which gives the change in the instantaneous entropy of the process.

Let us observe the similarity between (122,123) and (135,132); $\exp(-\mathbf{Z}_s^{h,t}[x])$ and $\exp(-\mathbf{W}_0^T[x])$ are exponential functionals of the Markov process. However $\exp(-\mathbf{W}_0^T[x])$ is not a forward martingale in the generic case because (135) implies that

$$\mathbf{E}_{0,y}\left[\exp(-\mathbf{W}_0^T)\right] = \frac{\int dx\rho_0^r(x)P_0^{r,T}(x,y)}{\rho_0(y)}. \tag{136}$$

Moreover,

$$\exp(-\mathbf{W}_0^0)(y) = \frac{\rho_0^r(y)}{\rho_0(y)}, \tag{137}$$

and then $\mathbf{E}_{0,y}[\exp(-\mathbf{W}_0^T)] \neq \exp(-\mathbf{W}_0^0)(y)$, except in the case where ρ_0^r is an invariant density of the backward dynamics. The fact that $\exp(-\mathbf{W}_0^T[x])$ is not a forward martingale does not prevent us from obtaining the Jarzynski equality [19, 49],

$$\left\langle\exp(-\mathbf{W}_0^T)\right\rangle = 1, \tag{138}$$

which is a direct subcase of (133). We will show in the next section that there is nevertheless a martingale interpretation of the action functional and the Jarzynski equality is one of its consequences.

The Jarzynski relation (138) implies two important results. First, the Jenssen inequality allows to obtain the Second Law of Thermodynamics,

$$\left\langle\mathbf{W}_0^T\right\rangle \geq 0. \tag{139}$$

Second, the Markov inequality [29] gives an upper bound on the probability of "transient deviations" from the Second Law:

$$\mathbf{P}\left(\exp\left(-\mathbf{W}_0^T\right) \geq \exp(L)\right) \leq \frac{\langle\exp(-\mathbf{W}_0^T)\rangle}{\exp(L)} \quad \text{then } \mathbf{P}\left(\mathbf{W}_0^T \leq -L\right) \leq \exp(-L). \tag{140}$$

6.2.2 Martingale Properties of the Action Functional

We noted in the last section that the functional $\exp(-\mathbf{W}_0^T)$ is not a martingale with respect to the time T of inversion. In order to unravel its links with the martingale theory, we shall define a functional similar to $\mathbf{W}_0^T$, but with a lower time indices different from 0 and a upper time indices different from T. This will be done through the comparison of the trajectorial measure $M_{\mu_0,[s,t]}$ for the forward system on the subinterval $[s,t]$ of $[0,T]$ and the push forward by the time inversion $R_*(M^r_{\mu_0^r,[T-t,T-s]})$ of the trajectorial measure for the backward system on the sub interval $[T-t, T-s]$[15]

$$R_*\left(M^r_{\mu_0^r,[T-t,T-s]}\right) = \exp\left(-\mathbf{W}_s^t\right) M_{\mu_0,[s,t]}. \tag{141}$$

Proceeding as in the last section (133), we can write the Crooks-type theorem for all functional $F_{[s,t]}$ of the trajectories from s to t,

$$\left\langle F_{[s,t]} \circ R\right\rangle^r = \left\langle F_{[s,t]} \exp\left(-\mathbf{W}_s^t\right)\right\rangle, \tag{142}$$

or, equivalently,

$$\begin{aligned} &\rho^r_{T-t}(x)\mathbf{E}^r_{T-t,x}\left[F_{[s,t]} \circ R[x]\delta(x_{T-s}-y)\right] \\ &\quad = \rho_s(y)\mathbf{E}_{s,y}\left[F_{[s,t]}[x]\exp\left(-\mathbf{W}_s^t[x]\right)\delta(x_t - x)\right], \end{aligned} \tag{143}$$

with $\rho_s^r(x) = \int dy \rho_0^r(y) P_0^{r,s}(y,x)$ and $\rho_s(x) = \int dy \rho_0(y) P_0^s(y,x)$. Finally, this includes also a Jarzynski type relation (138):[16]

$$\left\langle \exp(-\mathbf{W}_s^t)\right\rangle = 1. \tag{144}$$

For studying the martingale properties of $\exp(-\mathbf{W}_s^t)$, it is important to note that this functional is not strictly multiplicative. For $0 \le s \le u \le t \le T$, the Markov properties[17] imply the "multiplicative" law for the action functional:

$$\exp\left(-\mathbf{W}_s^t[dx]\right) = \exp\left(-\mathbf{W}_s^u[dx]\right)\exp\left(-\mathbf{W}_u^t[dx]\right)\frac{\rho_u}{\rho^r_{T-u}}(x_u). \tag{145}$$

This allows to introduce two functionals,

$$\mathbf{A}_s^t[dx] \equiv \frac{\rho_s}{\rho^r_{T-s}}(x_s)\exp\left(-\mathbf{W}_s^t[dx]\right) \quad \text{and} \quad \mathbf{R}_s^t[dx] \equiv \exp\left(-\mathbf{W}_s^t[dx]\right)\frac{\rho_t}{\rho^r_{T-t}}(x_t) \tag{146}$$

[15] Then the two measures deal with the "same part" of the trajectory.

[16] Note that $\exp(-\mathbf{W}_s^s)(y) = \frac{\rho^r_{T-s}(y)}{\rho_s(y)}$ and this seems to contradict (137) in the limit $s \to 0$. The resolution of the paradox is that expression here is obtained by the limit at fixed T: $\lim_{s\to 0}\lim_{t\to s}\mathbf{W}_s^t$, while (137) results from a different limiting procedure: $\lim_{T\to 0}\lim_{s\to 0}\mathbf{W}_s^T$.

[17]

$$M_{\mu_0,[s,t]}[dx] = \frac{M_{\mu_0,[s,u]}[dx]M_{\mu_0,[u,t]}[dx]}{\rho_u(x_u)dx_u},$$

and

$$R_*\left(M^r_{\mu_0^r,[T-t,T-s]}\right)[dx] = \frac{R_*(M^r_{\mu_0^r,[T-t,T-u]})[dx]R_*(M^r_{\mu_0^r,[T-u,T-s]})[dx]}{\rho^r_{T-u}(x_u)dx_u},$$

where the right hand sides describe the disintegration of the left-hand-side measures with respect to the map evaluating trajectories at time u.

with the strict multiplicative property:

$$\mathbf{A}_s^t = \mathbf{A}_s^u \mathbf{A}_u^t \quad \text{and} \quad \mathbf{R}_s^t = \mathbf{R}_s^u \mathbf{R}_u^t. \tag{147}$$

For these two functionals, the relation (143) implies that

$$\mathbf{E}_{s,y}\left[\mathbf{A}_s^t[x]\delta(x_t - x)\right] = \frac{\rho_{T-t}^r(x)}{\rho_{T-s}^r(y)} \mathbf{E}_{T-t,x}^r\left[\delta(x_{T-s} - y)\right], \tag{148}$$

and

$$\mathbf{E}_{s,y}\left[\mathbf{R}_s^t[x]\delta(x_t - x)\right] = \frac{\rho_t(x)}{\rho_s(y)} \mathbf{E}_{T-t,x}^r\left[\delta(x_{T-s} - y)\right], \tag{149}$$

yielding the Jarzynski-type relations,

$$\mathbf{E}_{s,y}\left[\mathbf{A}_s^t\right] = 1, \tag{150}$$

and

$$\left\langle \mathbf{R}_s^t[x]\delta(x_t - x)\right\rangle = \rho_t(x), \quad \text{i.e. } \mathbf{E}\left(\mathbf{R}_s^t | x_t = x\right) = 1. \tag{151}$$

Then, by using the multiplicative property (147) and the relation (150), we see that $\mathbf{R}_s^t$ is a forward martingale with respect to the natural filtration $\mathscr{F}_t$,

$$\mathbf{E}\left[\mathbf{A}_s^t | \mathscr{F}_u\right] = \mathbf{A}_s^u, \tag{152}$$

for $s \le u \le t$. Similarly, by using the multiplicative property (147) and the relation (151), we see that $\mathbf{R}_s^t$ is a backward martingale[18] with respect to the filtration $\mathscr{G}_s = \sigma(x_v, v \ge s)$ which describes the future of the process,

$$\mathbf{E}\left[\mathbf{R}_s^t | \mathscr{G}_u\right] = \mathbf{R}_u^t, \tag{153}$$

for $s \le u \le t$. From the definition (146), we deduce that the action functional $\exp(-\mathbf{W}_s^t)$ with $0 \le s \le u \le t < T$ is a forward martingale with respect to upper indices t[19] **and** a backward martingale with respect to lowest indices s.

This gives a martingale interpretation of the Jarzynski equality (138,144). One possible application is to improving the upper bound of the probability of "transient deviations" of the Second Law. The Doob inequality [24, 29] for forward martingales gives a stronger upper bound than the Markov inequality (140),

$$\mathbf{P}\Big(\sup_{t \text{ with } 0 \le s \le t \le T} \big(\exp\big(-\mathbf{W}_s^t\big)\big) \ge \exp(L)\Big) \le \frac{\langle \exp(-\mathbf{W}_s^t)\rangle}{\exp(L)}, \tag{154}$$

and then we obtain the relation

$$\mathbf{P}\Big(\inf_{t \text{ with } 0 \le s \le t \le T} \mathbf{W}_s^t \le -L\Big) \le \exp(-L). \tag{155}$$

[18] A backward martingale [24, 29] is dual to forward martingale, in the sense that its expectation in the past, given the knowledge accumulated in the future, is its present value.

[19] This is a little tricky because we proved in the last section that $\exp(-\mathbf{W}_s^T)$ is not a forward martingale with respect to T. What happens for $t = T$ is that a change of T implies also a change of the time inversion R which breaks the martingale property.

6.2.3 Action Functional $\mathbf{W}_s^t$ and the Time Reversed Process

It is proved in the probability literature [16, 31, 34, 44, 71, 72] that the time-reversed process, $RX_t \equiv X_{t^*}$ (with $t^* = T - t$), is also a Markov process. By using the results of Sect. 2.2, and more specifically, the expression of the cogenerator, (18), we can deduce that the Markov generator of the time-reversed process is

$$L_t^{CR} = L_{t^*}^* \equiv \rho_{t^*}^{-1} \circ L_{t^*}^\dagger \circ \rho_{t^*} - \rho_{t^*}^{-1} L_{t^*}^\dagger[\rho_{t^*}]\mathscr{I}. \tag{156}$$

Choosing this process as the backward process was called complete reversal in [11], and this explains the index "CR" on the left hand side. We remark that the instantaneous density of the time-reversed system is related to that of the original system by $\rho_t^{CR} \equiv \rho_{t^*}$. Denoting by $M^{r\circ CR}_{\mu_0,[s,t]}$ the trajectorial measure of the time reversal of the backward process initially distributed with the measure μ_0^r, we have the tautological formula:

$$R_*\left(M^r_{\mu_0^r,[T-t,T-s]}\right) = M^{r\circ CR}_{\mu_T^r,[s,t]}. \tag{157}$$

This allows to obtain an expression for the action functional $\mathbf{W}_s^t$ from (141) without push-forward R_*:

$$M^{r\circ CR}_{\mu_T^r,[s,t]} = \exp\left(-\mathbf{W}_s^t\right) M_{\mu_0,[s,t]}. \tag{158}$$

This expression will be used in the next section, but it also allows an easy proof of the assertion that $\exp(-\mathbf{W}_s^t)$ is a forward martingale in t and a backward martingale in s.

6.2.4 Class of Action Functional $\mathbf{W}_s^t$ (141) Which Are in Relation with the Exponential Martingale $\mathbf{Z}_s^t$ (119)

We consider here the case where the backward process is given by the generalized Doob f-transform of the adjoint generator $L^\dagger$ composed with an inversion of the time:

$$L_{u^*}^{r,f} = f_u^{-1} \circ L_u^\dagger \circ f_u - f_u^{-1} L_u^\dagger[f_u]; \quad u^* = T - u. \tag{159}$$

We shall denote by $\mathbf{W}_s^{f,t}$ the action functional associated with this choice of the backward process.

Using the definition of the total inversion (156) and after some algebra, one may show that

$$\left(L_u^{r,f}\right)^{CR} = \left(\rho_{u^*}^r\right)^{-1} f_u \circ L_u \circ \rho_{u^*}^r f_u^{-1} - \left(\rho_{u^*}^r\right)^{-1} f_u L_u[\rho_{u^*}^r f_u^{-1}]\mathcal{I}. \tag{160}$$

So, for $h_u \equiv \rho_{u^*}^r f_u^{-1}$, we have

$$\left(L_u^{r,f}\right)^{CR} = L_u^h, \tag{161}$$

upon using the definition of the generalized Doob h-transform (76).

Finally, by comparing the relations (158) and (123), we find the link between the two families of functionals:[20]

$$\exp\left(-\mathbf{W}_s^{f,t}\right) = \frac{\rho_{s^*}^r}{\rho_s}(x_s)\exp\left(-\mathbf{Z}_s^{h,t}\right), \tag{162}$$

[20] Note that $\rho_s^h = \rho_{s^*}^r$.

with $h_u \equiv \rho^r_{u*} f_u^{-1}$. Moreover, this relation allows to obtain from (119) an explicit expression for $\exp(-\mathbf{W}_s^{f,t})$:

$$\begin{aligned}\exp\left(-\mathbf{W}_s^{f,t}\right) &= \frac{\rho^r_{s*}}{\rho_s h_s}(x_s)\exp\left(-\int_s^t du\left(h_u^{-1}L_u\left[h_u\right]+h_u^{-1}\partial_u h_u\right)(x_u)\right)h_t(x_t)\\ &= \frac{f_s}{\rho_s}(x_s)\exp\left(-\int_s^t du\left(h_u^{-1}L_u\left[h_u\right]+h_u^{-1}\partial_u h_u\right)(x_u)\right)\frac{\rho^r_{t*}}{f_t}(x_t)\\ &= \frac{f_s}{\rho_s}(x_s)\exp\left(-\int_s^t du\left(f_u^{-1}L_u^\dagger\left[f_u\right]-f_u^{-1}\left(\partial_u f_u\right)\right)\right)\frac{\rho^r_{t*}}{f_t}(x_t),\end{aligned} \tag{163}$$

with, as before, $\rho_s(x) = \int dy \rho_0(y) P_0^s(y, x)$ and $\rho^r_{t*}(x) = \int dy \rho^r_0(y) P_0^{r,t^*}(y, x)$.[21] In particular, the action functional with $s = 0$ and $t = T$, which results for the choice $\rho_0 = f_0$ and $\rho^r_0 = f_T$, is then

$$\mathbf{W}_0^{f,T} = \int_0^T du\big(f_u^{-1}L_u^\dagger[f_u] - f_u^{-1}(\partial_u f_u)\big). \tag{164}$$

The form (159) taken for the backward generator may be justified by showing that it allows to recover the forms of time inversion usually taken in the probability or physics literature.

– First, we remark that the usual Doob f-transform corresponds to the case where we take for f_t the PDF (8) of the forward process (i.e., $\partial_t f_t - L_t^\dagger.f_t = 0$). Then, we recognize using formula (18) that $L^r_{t*} = L^*_t$ and then this backward process is the one obtained from the original one by the "complete reversal" considered in Sect. 6.2.3. This implies with (19) that

$$\begin{aligned}P_s^{*t} &= \overrightarrow{\exp}\left(\int_s^t du\big(L_u^*\big)^\dagger\right) = \overrightarrow{\exp}\left(\int_s^t du\big(L_{u^*}^{CR}\big)^\dagger\right)\\ &= \overrightarrow{\exp}\left(\int_{t^*}^{s^*} du\big(L_u^{CR}\big)\right)^\dagger = \big(P_{t^*}^{s^*,CR}\big)^\dagger.\end{aligned} \tag{165}$$

Finally, with (16), we obtain the generalized detailed balance,

$$\rho_s(x)P_s^t(x, y) = \rho_t(y)P_{t^*}^{s^*,CR}(y, x). \tag{166}$$

[21] The last equality in (163) results from the following algebra:

$$\begin{aligned}h_u^{-1}\partial_u h_u &= \left(\rho^r_{u*}\right)^{-1} f_u\partial_u\left(\rho^r_{u*}f_u^{-1}\right)\\ &= -f_u^{-1}\partial_u f_u + \left(\rho^r_{u*}\right)^{-1}\partial_u\left(\rho^r_{u*}\right)\\ &= -f_u^{-1}\partial_u f_u - \left(\rho^r_{u*}\right)^{-1}\left(L_{u^*}^{r,f}\right)^\dagger\left[\rho^r_{u*}\right]\\ &= -f_u^{-1}\partial_u f_u + f_u^{-1}L_u^\dagger[f_u] - \left(\rho^r_{u*}\right)^{-1} f_u L_u\left[\rho^r_{u*}f_u^{-1}\right].\end{aligned}$$

One may show that $\rho_t^{CR} \equiv \rho_{t^*}$ is the instantaneous density of the backward process and that the corresponding current operator (20) satisfies the relation

$$J_t^{CR} = -J_{t^*}, \tag{167}$$

which is very satisfying physically. This choice, however, corresponds to the vanishing of the functional $\mathbf{W}_s^t$ and of the entropy creation (equal to it due to the choice $\rho_0^{CR} = \rho_T$).

– Another useful choice of time inversion, called the current reversal in [10, 11], is based on the choice $f_t = \pi_t$, where π_t is the accompanying density (13). One can show that $\pi_t^r \equiv \pi_{t^*}$ is then the accompanying density for the backward process. If we associate with the accompanying density the current operator, by analogy with (20),

$$J_t \equiv \pi_t \circ L_t - L_t^\dagger \circ \pi_t, \tag{168}$$

we can easily show that still $J_t^r = -J_{t^*}$. The functional (163) now takes the form

$$\exp\left(-\mathbf{W}_s^{f=\pi,t}\right) = \frac{\pi_s}{\rho_s}(x_s)\exp\left(\int_s^t du(\partial_u \ln \pi_u)(x_u)\right)\left(\frac{\pi_t}{\rho_{T-t}^r}\right)^{-1}(x_t). \tag{169}$$

Moreover, the choice of initial density $\rho_0 = \pi_0$ and $\rho_0^r = \pi_0^r = \pi_T$, implies that

$$\mathbf{W}_0^{f=\pi,T} = -\int_0^T (\partial_u \ln \pi_u)(x_u)\, du \equiv \mathbf{W}_0^{T,ex}, \tag{170}$$

where the index "ex" stands for "excess" [11, 75, 82]. The Jarzynski equality (138) for this case was first proved for a one-dimensional diffusion process in [43] and then for Markov chains [15, 37], general diffusion processes [11, 62], and pure jump processes [63]. We see here that these **FR** are true for general Markov processes, including stochastic equation with Poisson noise (52) or with Levy noise. This is an optimistic result for the generality of **FR** in the context of the proof in [6, 89] that the Gallavotti-Cohen relation for the work is broken for a particle in a harmonic potential subject to a Poisson or Levy noise. Moreover, in the case of the jump Langevin equation (63), we have the normalized accompanying density $\pi_t = \exp(-\beta(H_t - F_t))$ (where F_t is the free energy) and then

$$\mathbf{W}_0^{T,ex} = \beta \int_0^T (\partial_u H_u)(x_u)\, du - \beta(F_T - F_0). \tag{171}$$

So, in this case, the finite time **FR** (133) for the dissipative work performed on the system is valid.

– For diffusion processes, it was shown in [11] that to obtain a sufficiently flexible notion of time inversion, we should allow for a non-trivial behavior of the modified drift $\widehat{u}_t$ (see [11]) under the time-inversion by dividing it into two parts:

$$\widehat{u}_t = \widehat{u}_{t,+} + u_{t,-}. \tag{172}$$

Here $\widehat{u}_{t,+}$ transforms as a vector field under time inversion, i.e., $\widehat{u}_{t^*,+}^r = +\widehat{u}_{t,+}$, while $u_{t,-}$ transforms as a pseudo-vector field, i.e., $u_{t^*,-}^r = -u_{t,-}$. The random field η_t may be transformed with either of the two rules: $\eta_{t^*}^r = \pm\eta_t$. It can be shown [14] that the choice of the vector field part which allows us to obtain the backward generator given by (159) is

$$\widehat{u}_{t,+} = \frac{d_t}{2}\nabla(\ln f_t). \tag{173}$$

This is the choice made to obtain formula (22) in [14] in order to find **FR** that are global versions of **GFDT** in the context of a Langevin process, and we find (164) as formula (24) in [14].

6.2.5 *Fluctuation-Dissipation Theorem as Taylor Expansion of Fluctuation Relation for the Class of Functional* $\exp(-\mathbf{W}_s^{f,t})$

For completeness, we recall here the proof, done in [14] for a diffusion process, that the family of **FR** (133) with (164) are also global versions of the **GFDT** (91,94). More precisely, they are global versions of the fundamental relation of the linear response theory (75) which, as explained in Sect. 5.3, implies the **GFDT** (91, 94).

For the dynamics of the perturbed systems (76), we consider the fluctuation relation (133) with the functional (164) written for f_t (with $f_t(x) = 1 + k_t A_t(x) + O(k^2)$) as the mean instantaneous density ρ_t of the unperturbed system (with $f = 1 \equiv k = 0$). The functional (164) becomes

$$\mathbf{W}_0^{f,T} = \int_0^T k_s\big({\rho_s}^{-1} N_s^\dagger[\rho_s]]\big)(x_s)\,ds, \tag{174}$$

where N is defined in (74) . Let us now write a particular case of (133) for a single time functional $F[x] = A^a(x_t) \equiv A_t^a$ $(0 < t < T)$:

$$\big\langle A_t \exp\big(-\mathbf{W}_0^{f,T}\big)\big\rangle^f = \langle A_{T-t}\rangle^{f,r}. \tag{175}$$

The first order Taylor expansion,

$$\exp\big(-\mathbf{W}_0^{f,T}\big) = 1 + \int_0^T k_s\,\big((\rho_s^{-1} N_s^\dagger[\rho_s]\big)\,(x_s)\,ds + \mathcal{O}(k^2), \tag{176}$$

in (175) gives the relation

$$\begin{aligned}\big\langle A_t\big\rangle + \int k_s \frac{\delta}{\delta k_s}\bigg|_{k=0} \langle A_t\rangle^f\ ds - \int_0^T k_s\,\big\langle {\rho_s}^{-1} N^\dagger[\rho_s](x_s) A_t(x_t)\big\rangle ds + \mathcal{A}(k^2)\\ = \big\langle A_{T-t}\big\rangle^{f,r}.\end{aligned} \tag{177}$$

Due to the form of the considered inversion (159), the right hand side has a functional dependence only on $\{k_{T-u}, T-u < T-t\}$, i.e. on $\{k_u, u > t\}$. So, if we apply $\frac{\delta}{\delta k_s}|_{k=0}$ for $0 < s \le t$ to the last identity, we obtain the relation (75).

7 Conclusions

We have shown that the kinematics of a Markov process, namely, the local velocity (25,26,27) and the derivatives (28), allow to develop a unified approach to obtain recent **GFDT** in the context of fairly general Markovian evolutions (Sect. 5.3). We have also elucidated the form of the usual perturbation (76) used for **FDT** by showing its similarity to the Doob h-transform well known in the probabilistic literature. We also presented examples where the physical perturbation is more general, e.g. given by a time change (110) or by a thermal perturbation (Sect. 5.4.3). We derived the **GFDT** for these examples (111,112,116). In this paper, we have also presented a class of the exponential martingale functionals (119), which represents an alternative to **FR** as a non-perturbative extension of **GFDT** (Sect. 6.1.3). Moreover, we established in Sect. 6.2.4 a direct link between this family of functionals and the **FR**. We showed that the **FR** also involve a family of martingales which for a fairly general class of **FR**, including several classes discussed in the literature, coincides with exponential martingales. This class of **FR** was obtained by comparison of the original Markov process to the backward process whose generators (159) are generalized Doob transforms for the adjoints of the original generators. In the process, we improved the classical upper bound for "transient deviations" from the Second Law (155). Our hope is that, despite lack of rigor from the mathematical perspective, this article will serve as a bridge between nonequilibrium physics and probability theory.

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Appendix A: Proof of the Relation (35)

By taking the derivative of the relation (34) with respect to t $(> s)$, we get

$$\begin{aligned}\partial_t\big\langle U_s(x_s)V_t(x_t)\big\rangle &= \int dxdyU_s(x)\rho_s(x)\big(\partial_t P_s^t(x,y)\big)V_t(y)\\ &\quad+\int dxdyU_s(x)\rho_s(x)P_s^t(x,y)\big(\partial_t V_t(y)\big)\\ &=\big\langle U_s(x_s)\big(\partial_t V_t+L_t(V_t)\big)(x_t)\big\rangle=\bigg\langle U_s(x_s)\frac{d_+V_t}{dt}(x_t)\bigg\rangle.\end{aligned}$$

In deriving the second line, we use the forward Kolmogorov equation (5). Now, by taking the derivative of (34) with respect to s $(< t)$, and by using the definition of the cogenerator (19), we get

$$\begin{aligned}&\partial_s\big\langle U_s(x_s)V_t(x_t)\big\rangle\\ &\quad=\int dxdyU_s(x)\big(\partial_s P_s^{*t}(x,y)\big)\rho_t(y)V_t(y)+\int dxdy\big(\partial_s U_s(x)\big)P_s^{*t}(x,y)\rho_t(y)V_t(y)\\ &\quad=-\int dxdyU_s(x)\big(\big(L_s^*\big)^\dagger P_s^{*t}\big)(x,y)\rho_t(y)V_t(y)\\ &\qquad+\int dxdy\big(\partial_s U_s(x)\big)P_s^{*t}(x,y)\rho_t(y)V_t(y)\\ &\quad=-\int dxdydzU_s(x)L_s^*(z,x)P_s^{*t}(z,y)\rho_t(y)V_t(y)\\ &\qquad+\int dxdy\big(\partial_s U_s(x)\big)P_s^{*t}(x,y)\rho_t(y)V_t(y)\\ &\quad=-\int dydz\big(L_s^*U_s\big)(z)P_s^{*t}(z,y)\rho_t(y)V_t(y)+\int dxdy\big(\partial_s U(s,x)\big)P_s^{*t}(x,y)\rho_t(y)V_t(y)\end{aligned}$$

$$= \left\langle \left(\partial_s U_s - L_s^* U_s\right)(x_s) V_t(x_t) \right\rangle = \left\langle \frac{d_- U_s}{ds}(x_s) V_t(x_t) \right\rangle.$$

Appendix B: Proof of the Relation (47)

The formal adjoint of the generator (42) of a diffusion process is given by

$$L_t^\dagger = -\nabla_i \circ \widehat{u}_t^i + \frac{1}{2} \nabla_i \circ d_t^{ij} \circ \nabla_j .$$

So, for all functions f_t in $\mathscr{E}$, we can express the operator $f_t^{-1} \circ L_t^\dagger \circ f_t$ as

$$\begin{aligned}
& f_t^{-1} \circ L_t^\dagger \circ f_t \\
&\quad = f_t^{-1} \circ \left(-\nabla_i \circ \widehat{u}_t^i + \frac{1}{2} \nabla_i \circ d_t^{ij} \circ \nabla_j \right) \circ f_t \\
&\quad = f_t^{-1} \circ \left(-\left(\nabla_i \left(\widehat{u}_t^i f_t\right)\right) - \widehat{u}_t^i f_t \circ \nabla_i + \frac{1}{2} \nabla_i \circ \left(d_t^{ij} (\nabla_j f_t) + f_t d_t^{ij} \circ \nabla_j \right) \right) \\
&\quad = f_t^{-1} \Bigg(-\left(\nabla_i \left(\widehat{u}_t^i f_t\right)\right) - \widehat{u}_t^i f_t \circ \nabla_i + \frac{1}{2} \nabla_i \left(d_t^{ij} \nabla_j f_t \right) + \frac{d_t^{ij}}{2} (\nabla_j f_t) \circ \nabla_i \\
&\qquad + \frac{d_t^{ij}}{2} (\nabla_i f_t) \circ \nabla_j + \frac{f_t}{2} \nabla_i \circ d_t^{ij} \circ \nabla_j \Bigg) \\
&\quad = f_t^{-1} L_t^\dagger [f_t] + L_t - 2 \left(\widehat{u}_t^i - \frac{d_t^{ij}}{2} (\nabla_j \ln f_t) \right) \nabla_i .
\end{aligned} \tag{178}$$

Moreover, with $f_t = \rho_t$ (PDF (8)) and with (9), we obtain

$$\rho_t^{-1} \circ L_t^\dagger \circ \rho_t - \rho_t^{-1} (\partial_t \rho_t) = L_t - 2 \left(\widehat{u}_t^i - \frac{d_t^{ij}}{2} (\nabla_j \ln \rho_t) \right) \nabla_i .$$

By using the definition of the cogenerator (18) and of the **hydrodynamic velocity** (45), we obtain the formula (47).

Appendix C: Proof of the Relation (75)

We start with the first-order Dyson expansion [52] of the ordered exponential (4):

$$\begin{aligned}
\overrightarrow{\exp}\left(\int_0^t du (L_u + k_u N_u) \right) &= \overrightarrow{\exp}\left(\int_0^t du L_u \right) \\
&\quad + \int_0^t ds \overrightarrow{\exp}\left(\int_0^s du L_u \right) k_s N_s \overrightarrow{\exp}\left(\int_s^t ds L_s \right) + O(k^2).
\end{aligned}$$

Then, for the one point functional, one has

$$\left\langle A_t(x_t)\right\rangle' = \int dxdy\rho_0(x)P_0^t(x,y)A_t(y) + \int_0^t dsk_s\int dxdydzdz'\rho_0(x)P_0^s(x,y)N_s(y,z)P_s^t\big(z,z'\big)A_t\big(z'\big) + O\big(k^2\big).$$

The response function is then given by

$$\begin{aligned}\left.\frac{\delta\langle A_t(x_t)\rangle'}{\delta k_s}\right|_{k=0} &= \int dxdydzdz'\rho_0(x)P_0^s(x,y)N_s(y,z)P_s^t\big(z,z'\big)A_t\big(z'\big)\\ &= \int dydzdz'\rho_s(y)N_s(y,z)P_s^t\big(z,z'\big)A_t\big(z'\big)\\ &= \int dzdz'\big(N_s^\dagger\rho_s\big)(z)P_s^t\big(z,z'\big)A_t\big(z'\big).\end{aligned}$$

which is (75).

Appendix D: Proof of the Relation (80)

With the formula (42) for the generator of a diffusion process, and for two arbitrary functions f and g on $\mathscr{E}$, one has

$$\begin{aligned}L_t[fg] &= \widehat{u}_t^i\nabla_i[fg] + \frac{1}{2}\big(\nabla_i\circ d_t^{ij}\circ\nabla_j\big)[fg] = f\widehat{u}_t^i(\nabla_i g) + \widehat{u}_t^i(\nabla_i f)g\\ &\quad + \frac{1}{2}\nabla_i\big(d_t^{ij}(\nabla_j f)g + d_t^{ij}f(\nabla_j g)\big)\\ &= f\widehat{u}_t^i(\nabla_i g) + \widehat{u}_t^i(\nabla_i f)g + \frac{1}{2}\big(\nabla_i\big(d_t^{ij}\nabla_j f\big)\big)g + d_t^{ij}(\nabla_j f)(\nabla_i g) + \frac{f}{2}\big(\nabla_i\big(d_t^{ij}\nabla_j g\big)\big)\\ &= fL_t(g) + L_t(f)g + d_t^{ij}(\nabla_i f)(\nabla_j g).\end{aligned}$$

We then obtain the formula (80) for the operator "carre du champs":

$$\Gamma_t(f,g) = d_t^{ij}(\nabla_i f)(\nabla_j g).$$

Appendix E: Proof of the Relation (118)

We start by proving the operatorial relation

$$P_s^{h,t} = h_s^{-1}\overrightarrow{\exp}\left(\int_s^t du\big(L_u - h_u^{-1}L_u[h_u] - h_u^{-1}\partial_u h_u\big)\right)h_t.$$

First, it is easy to see that the above relation is true when $t=s$ (also, then both the left hand side and the right hand side equal the identity). Moreover, we now show that the two sides of the relation verify the same differential equation. For example, the right hand side satisfies

$$\partial_t\left(h_s^{-1}\overrightarrow{\exp}\left(\int_s^t du\big(L_u - h_u^{-1}L_u[h_u] - h_u^{-1}\partial_u h_u\big)\right)h_t\right)$$

$$= h_s^{-1}\overrightarrow{\exp}\left(\int_s^t du\big(L_u - h_u^{-1}L_u[h_u] - h_u^{-1}\partial_u h_u\big)\right)\circ\big(L_t\circ h_t - L_t(h_t) - \partial_t h_t + \partial_t h_t\big)$$

$$= \left(h_s^{-1}\overrightarrow{\exp}\left(\int_s^t du\big(L_u - h_u^{-1}L_u[h_u] - h_u^{-1}\partial_u h_u\big)\right)h_t\right)\circ\big(h_t^{-1}\circ L_t\circ h_t - h_t^{-1}L_t(h_t)\big)$$

$$= \left(h_s^{-1}\overrightarrow{\exp}\left(\int_s^t du\big(L_u - h_u^{-1}L_u[h_u] - h_u^{-1}\partial_u h_u\big)\right)h_t\right)\circ L_t^h.$$

It is easy to see by using the forward Kolmogorov equation that the right hand side verifies the same equation. Now, we can apply the Feynman-Kac formula [79, 87] to the right hand side of (E), and we obtain the relation (118), namely,

$$P_s^{h,t}(x,y) = \mathbf{E}_{s,x}\big(\delta(x_t - y)\exp\big(-\mathbf{Z}_s^{h,t}[x]\big)\big),$$

with the functional $\exp(-\mathbf{Z}_s^t[x])$ given by the relation (119).

Appendix F: Proof of the Relation (122)

We now want to prove the relation (122) with F an arbitrarily functional of the trajectories on $[s,t]$. It suffices to check this identity for the so-called cylindrical functional:

$$F_{[s,t]}[x] = F(x_s, x_{t_1}, x_{t_2}, \ldots, x_{t_n}, x_t) \text{ for } s \le t_1 \le t_2 \le \cdots \le t_n \le t.$$

We will use the Markov structure of the trajectory measure.

$$\mathbf{E}_{s,x}^h\big[F(x_s, x_{t_1}, x_{t_2}, \ldots, x_{t_n}, x_t)\big]$$

$$= \int dx_1 dx_2 \ldots dx_n dy\, F(x, x_1, x_2, \ldots, x_n, y) P_s^{h,t_1}(x, dx_1) P_{t_1}^{h,t_2}(x_1, dx_2) \ldots P_{t_n}^{h,t}(x_n, y)$$

$$= \int dx_1 dx_2 \ldots dx_n dy\, F(x, x_1, x_2, \ldots, x_n, y) h_s^{-1}(x)$$

$$\times\, \mathbf{E}_{s,x}\left[\delta(x_{t_1} - x_1)\exp\left(-\int_s^{t_1} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\right)\right] h_{t_1}(x_1) h_{t_1}^{-1}(x_1)$$

$$\times\, \mathbf{E}_{t_1,x_1}\left[\delta(x_{t_1} - x_2)\exp\left(-\int_{t_1}^{t_2} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\right)\right]\ldots$$

$$\times\, \mathbf{E}_{t_n,x_n}\left[\delta(x_t - y)\exp\left(-\int_{t_n}^{t} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\right)\right] h_t(y)$$

$$= \int dx_1 dx_2 \ldots dx_n dy\, F(x, x_1, x_2, \ldots, x_n, y) h_s^{-1}(x) E_{s,x}$$

$$\times \left[\delta(x_{t_1} - x_1)\exp\left(-\int_s^{t_1} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\right)\right]$$

$$\times\, \mathbf{E}_{t_1,x_1}\left[\delta(x_{t_1} - x_2)\exp\left(-\int_{t_1}^{t_2} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\right)\right]\ldots$$

$$\times \mathbf{E}_{t_n,x_n}\Big[\delta(x_t - y)\exp\Big(-\int_{t_n}^{t} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\Big)\Big]h_t(y)$$

$$= \mathbf{E}_{s,x}\Big[F(x_s, x_{t_1}, x_{t_2}, \ldots, x_{t_n}, x_t)h_s^{-1}(x_s)$$

$$\times \exp\Big(-\int_{s}^{t} du\big(h_u^{-1}L_u(h_u) + h_u^{-1}\partial_u h_u\big)\Big)h_t(x_t)\Big]$$

$$= \mathbf{E}_{s,x}\big[F_{[s,t]}\exp\big(-\mathbf{Z}_s^{h,t}[x]\big)\big].$$

We thus arrive at (122).

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