

Fluctuation Relations for Diffusion Processes

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Abstract: The paper presents a unified approach to different fluctuation relations for classical nonequilibrium dynamics described by diffusion processes. Such relations compare the statistics of fluctuations of the entropy production or work in the original process to the similar statistics in the time-reversed process. The origin of a variety of fluctuation relations is traced to the use of different time reversals. It is also shown how the application of the presented approach to the tangent process describing the joint evolution of infinitesimally close trajectories of the original process leads to a multiplicative extension of the fluctuation relations.

1. Introduction

Nonequilibrium statistical mechanics attempts a statistical description of closed and open systems evolving under the action of time-dependent conservative forces or under time-independent or time dependent non-conservative ones. **Fluctuation relations** are robust identities concerning the statistics of entropy production or performed work in such systems. They hold arbitrarily far from thermal equilibrium. Close to equilibrium, they reduce to Green-Kubo or fluctuation-dissipation relations, usually obtained in the scope of linear response theory [87, 44]. Historically, the study of fluctuation relations originated in the numerical observation of Evans, Cohen and Morriss [23] of a symmetry in the distribution of fluctuations of microscopic pressure in a thermostatted particle system driven by external shear. The symmetry related the probability of occurrence of positive and negative time averages of pressure over sufficiently long time intervals and predicted that the former is exponentially suppressed with respect to the latter. Ref. [23] attempted to explain this observation by a symmetry, induced by the time-reversibility, of the statistics of partial sums of finite-time Lyapunov exponents in dissipative dynamical systems. This was further elaborated in [25] where an argument was given explaining

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such a symmetry in a transient situation when one starts with a simple state which evolves under dynamics, see also [26]. In refs. [35,36], Gallavotti and Cohen provided a theoretical explanation of the symmetry observed numerically in [23] employing the theory of uniformly hyperbolic dynamical systems. In this theory, the stationary states correspond to invariant measures of the SRB type [82] and the entropy production is described by the phase-space contraction [74]. The authors of [35,36] established a **fluctuation theorem** about the rate function describing the statistics of large deviations of the phase-space contraction in a time-reversible dynamics. To relate to the behavior of realistic systems, they formulated the **chaotic hypothesis** postulating that many such systems behave, for practical purposes, as the uniformly hyperbolic ones. They interpreted the numerical observations of ref. [23] as a confirmation of this hypothesis. The difference between the fluctuation relations for a transient situation analyzed in [25,26] and the stationary one discussed in [35,36] was subsequently stressed in [16]. The debate about the connection between the transient and stationary fluctuation relations still continues, see e.g. [77] and [33].

In another early development, Jarzynski established in [48] a simple transient relation for the statistics of fluctuations of work performed on a system driven by conservative time-dependent forces. This relation is now known under the name of the Jarzynski equality. A similar observation, but with more limited scope, was contained in earlier work [4–6], see [52] for a recent comparison. The simplicity of the Jarzynski equality and its possible applications to measurements of free-energy landscape for small systems attracted a lot of attention, see [72,73] and the references therein.

The first studies of fluctuation relations dealt with the deterministic dynamics of finitely-many degrees of freedom. Such dynamics may be also used to model systems interacting with environment or with heat reservoirs. To this end, one employs simplified finite-dimensional models of reservoirs forced to keep their energy constant [24]. This type of models was often used in numerical simulations and in discussing fluctuation relations, see e.g. [33]. A more realistic treatment of reservoirs would describe them as infinite systems prepared in the thermal equilibrium state. Up to now, only infinite systems of non-interacting particles could be treated effectively, see [21,22]. A less realistic description of interaction with environment or with reservoirs consists of replacing them by a random noise, usually shortly correlated in time. This leads to Markovian stochastic evolution equations. Stochastic models are often easier to control than deterministic ones and they became popular in modeling nonequilibrium dynamics.

In [49], Jarzynski generalized his relation to time-dependent Markov processes with the instantaneous generators satisfying the detailed balance relation. At almost the same time, Kurchan has shown in [56] that the stationary fluctuation relations hold for the stochastic Langevin-Kramers evolution. His result was extended to more general diffusion processes by Lebowitz and Spohn in [59]. In [63], Maes has traced the origin of fluctuation relations to the Gibbsian nature of the statistics of the dynamical histories, see a recent discussion of the fluctuation relations from this point of view in [64]. Searles and Evans generalized their transient fluctuation relation to the stochastic setup in [76]. Finally, within the stochastic approach, the scope of the transient fluctuation relations was further extended due to the works of Crooks [18,19], Jarzynski [51], Hatano and Sasa [46], Speck and Seifert [78] and Chernyak, Chertkov and Jarzynski [10], just to cite only the papers that most influenced the present authors. It is worth stressing that the general transient fluctuation relations do not impose the time reversibility of the dynamics but compare the fluctuation statistics of the original process and of its time reversal. Such an extension of the scope of fluctuation relations is a possibility in the

stationary case as well, but it becomes a necessity in many transient situations. Within the theory of the hyperbolic dynamical systems, the stationary fluctuation theorem of [35] was recently generalized to the random dynamics in [8].

In [1], Balkovsky, Falkovich and Fouxon noticed another robust relation concerning the large deviations of finite-time Lyapunov exponents in the context of homogeneous hydrodynamic flows. It was remarked in [29], that this observation, which we shall call, following [40], the **multiplicative fluctuation relation**, provides an extension of the previously known fluctuation relations for the phase-space contraction. The simple argument presented in [1] dealt with a transient situation. It was very similar to the original Evans-Searles argument as formulated later in [26]. The multiplicative fluctuation relation was explicitly checked in the Kraichnan model of hydrodynamic flows [1, 29, 11].

The theoretical work on fluctuation relations has established most of them as mathematical identities holding within precisely defined models, but concerning statistics of events that are rare, especially for macroscopic systems. The relevance of such identities to numerical simulations and, even more, to real experiments, required a confirmation. Numerical (see e.g. [7, 45, 83, 38, 86]) and experimental testing of the fluctuation relations (see e.g. [15, 37, 17, 2, 54, 47]) has attracted over the years a lot of attention, inspiring further developments. It will probably remain an active field in the future. It is not, however, the topic of the present paper.

The growing number of different fluctuation relations made urgent a development of a unifying approach. Several recent reviews partially provided such a unification from different points of view, see ref. [26, 64, 57, 10]. In the present paper, we attempt another synthesis, with the aim of supplying a uniform derivation of most of the known fluctuation relations, including the multiplicative ones. We shall work in the setup of (possibly non-autonomous) diffusion processes in finite-dimensional spaces, somewhat similar, but more general than the one adopted in [59]. The systems considered include, as special cases, the deterministic dynamics, the Langevin stochastic equation, and the Kraichnan model of hydrodynamic flow. This is certainly not the most general setup possible for discussing fluctuation relations (for example, the discrete-time dynamics, the stochastic dynamics with jumps, or non-Markovian evolutions are not covered), but it is general enough for a unified discussion of a variety of aspects of fluctuation relations. Most of our considerations are simple extensions of arguments that appeared earlier in usually more constrained contexts. There are two basic ideas that we try to exploit to obtain a larger flexibility than in the previous discussions of fluctuation relations. The first one concerns the possible time-reversed processes that we admit. This idea appeared already in [10], where two different time inversions were used for the Langevin dynamics with non-conservative forces, leading to two different backward processes and two different fluctuation relations. We try to exploit the freedom of choice of the time-inversion in a more systematic way. The second idea, which seems original to us, although it is similar in spirit to the first one, is to obtain new fluctuation relations by considering new diffusion processes derived from the original one. In particular, we show that the multiplicative fluctuation relations for general diffusion processes may be obtained by writing a more standard relation for the tangent diffusion process describing a simultaneous evolution of infinitesimally close trajectories of the original process. The same idea may be used [13] to explain additional fluctuation relations, like the one for the rate function of the difference of finite-time Lyapunov exponents “along unstable flag” that was observed in [11] for the anisotropic Kraichnan model.

The present paper is organized as follows. In Sect. 2, we define the class of diffusion processes that will be discussed and list four special cases. Section 3 recalls the notions of transition probabilities and generators of a diffusion process, as well as the detailed balance relation. In Sect. 4, we introduce the tangent diffusion process induced from the original one and define the phase-space contraction. Time inversions leading to different backward processes are discussed in Sect. 5, with few important examples listed in Sect. 6. A formal relation between the expectations in the forward and in the backward process is introduced in Sect. 7. As examples, we discuss the case of tangent process in the homogeneous Kraichnan flow, a simple generalization of the detailed balance relation and the 1st law of thermodynamics for the Langevin dynamics. Section 8 is devoted to a general version of the Jarzynski equality, whose different special cases are reviewed, and Sect. 9 to a related equality established by Speck and Seifert in [78]. We formulate the Jarzynski equality as a statement that for a certain functional \mathcal{W} of the diffusion process, the expectation value of $e^{-\mathcal{W}}$ is normalized. In Sect. 10, the functional \mathcal{W} is related to the entropy production and the positivity of its expectation value is interpreted as the 2nd law of thermodynamics for the diffusive processes. In Sect. 11, we show how the general Jarzynski equality reduces in the linear response regime to the Green-Kubo and Onsager relations for the transport coefficients and to the fluctuation-dissipation theorem. In Sect. 12, we discuss briefly a peculiar one-dimensional Langevin process in which the equilibrium is spontaneously broken and replaced by a state with a constant flux, leading to a modification of the fluctuation-dissipation relation. The model is well known from the theory of one-dimensional Anderson localization and describes also the separation of infinitesimally close particles with inertia carried by a one-dimensional Kraichnan flow. Section 13.3 formulates in the general setup of diffusion processes what is sometimes termed a detailed fluctuation relation [51,19], an extension of the Crooks fluctuation relations [18]. Few special cases are retraced in Sect. 14.

Up to this point of the paper, the discussion is centered on the transient evolution where the system is initially prepared in a state that changes under the dynamics. In Sect. 15, we discuss the relation of the transient fluctuation relations to the stationary ones which pertain to the situation where the initial state is preserved by the evolution. The stationary relations are usually written for the rate function of large deviations of entropy production observed in the long-time regime. In our case, they describe the long time asymptotics of the statistics of \mathcal{W} . The Gallavotti-Cohen relation was the first example of such identities. We show how the fluctuation relation for the tangent process in the homogeneous Kraichnan flow discussed in Sect. 7 leads to a generalization of the Gallavotti-Cohen relation that involves the large-deviations rate function of the so called stretching exponents whose sum describes the phase-space contraction. In Sect. 16, we extend such a multiplicative fluctuation relation to the case of general diffusion processes. Section 17 contains speculation about possible versions of fluctuation relations for multi-point motions and Sect. 18 collects our conclusions. Few simple but more technical arguments are deferred to Appendices in order not to overburden the main text, admittedly already much more technical than most of the work on the subject. Some of the technicalities are due to a rather careful treatment of the intricacies related to the conventions for the stochastic differential equations that are usually omitted in physical literature. The aim at generality, even without pretension of mathematical rigor, places the stress on the formal aspects and makes this exposition rather distant from physical discourse, although we make an effort to include many examples that illustrate general relations in more specific situations. The physical content is, however, more transparent in examples to such examples which are scarce in the present text but which abound in

the existing literature to which we often refer. Certainly, the paper will be too formal for many tastes, and we take precautions to warn the potential reader who can safely omit the more technical passages.

After submission of the first version of the paper, we received the article [66] which influenced our revision of Sect. 10.

2. Forward Process

As mentioned in the Introduction, the present paper deals with non-equilibrium systems modeled by diffusion processes of a rather general type. More concretely, the main objects of our study are the stochastic processes \mathbf{x}_t in \mathbf{R}^d (or, more generally, on a d -dimensional manifold), described by the differential equation

$$\dot{\mathbf{x}} = \mathbf{u}_t(\mathbf{x}) + \mathbf{v}_t(\mathbf{x}), \quad (2.1)$$

where $\dot{\mathbf{x}} \equiv \frac{d\mathbf{x}}{dt}$ and, on the right hand side, $\mathbf{u}_t(\mathbf{x})$ is a time-dependent deterministic vector field (a drift), and $\mathbf{v}_t(\mathbf{x})$ is a Gaussian random vector field with mean zero and covariance

$$\langle v_t^i(\mathbf{x}) v_s^j(\mathbf{y}) \rangle = \delta(t - s) D_t^{ij}(\mathbf{x}, \mathbf{y}). \quad (2.2)$$

Due to the white-noise nature of the temporal dependence of \mathbf{v}_t (typical \mathbf{v}_t are distributional in time), Eq. (2.1) is a stochastic differential equation (SDE). We shall consider it with the Stratonovich convention¹ [71, 67], keeping for the Stratonovich SDEs the notation of the ordinary differential equations (ODEs). Examples of systems described by Eq. (2.1) include four special cases that we shall keep in mind.

Example 1. Deterministic dynamics. Here $\mathbf{v}_t(\mathbf{x}) \equiv 0$ and $D_t^{ij}(\mathbf{x}, \mathbf{y}) \equiv 0$ so that Eq. (2.1) reduces to the ODE

$$\dot{\mathbf{x}} = \mathbf{u}_t(\mathbf{x}). \quad (2.3)$$

Example 2. Lagrangian flow in the Kraichnan model. This is a process used in modeling turbulent transport. The SDE (2.1), where one usually takes $\mathbf{u}_t(\mathbf{x}) \equiv 0$, describes the motion of tracer particles in a stationary Gaussian ensemble of velocities $\mathbf{v}_t(\mathbf{x})$ white in time. Such an ensemble, with an appropriate time-independent spatial covariance $D^{ij}(\mathbf{x}, \mathbf{y})$, was designed by Kraichnan [62] to mimic turbulent velocities. In particular, homogeneous flows are modeled by imposing the translation invariance $D^{ij}(\mathbf{x}, \mathbf{y}) = D^{ij}(\mathbf{x} - \mathbf{y})$ and isotropic ones by assuming that $D^{ij}(\mathbf{x}, \mathbf{y})$ is rotation-covariant. In this paper, we shall consider only the case when $D^{ij}(\mathbf{x}, \mathbf{y})$ is smooth. A discussion of the case with $D^{ij}(\mathbf{x}, \mathbf{y})$ non-smooth around the diagonal, pertaining to the fully developed turbulence, may be found in [29], or, on a mathematical level, in [60].

Example 3. Langevin dynamics. Here Eq. (2.1) takes the form²

$$\dot{\mathbf{x}}^i = -\Gamma^{ij} \partial_j H_t(\mathbf{x}) + \Pi^{ij} \partial_j H_t(\mathbf{x}) + G_t^i(\mathbf{x}) + \zeta_t^i, \quad (2.4)$$

¹ The choice of the Stratonovich convention guarantees that \mathbf{u}_t and \mathbf{v}_t transform as vector fields under a change of coordinates.

² We use throughout the paper the summation convention.

where Γ is a constant non-negative matrix and Π an antisymmetric one, the Hamiltonian H_t is a, possibly time dependent, function, G_t is an additional force, and ζ_t is the d -dimensional white noise with the covariance

$$\langle \zeta_t^i \zeta_s^j \rangle = 2 \delta(t-s) \beta^{-1} \Gamma^{ij}. \quad (2.5)$$

In this example, the noise ζ_t plays the role of the (space-independent) random vector field v_t so that $D_t^{ij}(x, y) = 2\beta^{-1}\Gamma^{ij}$. For $G_t \equiv 0$ and a time independent Hamiltonian $H_t \equiv H$, the Langevin dynamics is used to model the approach to thermal equilibrium at inverse temperature β [46]. The deterministic vector field $-\Gamma^{ij}\partial_j H$ drives the solution towards the minimum of H (if it exists) whereas the Hamiltonian vector field $\Pi^{ij}\partial_j H$ preserves H . The noise ζ_t generates thermal fluctuations of the solution. Note that its spatial covariance is aligned with the matrix Γ appearing in the dissipative force $-\Gamma^{ij}\partial_j H$ (such an alignment, known from Einstein's theory of Brownian motion, is often called the Einstein relation). Inclusion of the Hamiltonian vector field permits to model systems where the noise acts only on some degrees of freedom, e.g. the ones at the ends of a coupled chain, with the rest of the degrees of freedom undergoing a Hamiltonian dynamics. The introduction of a time-dependence and/or of the force G_t permits to model nonequilibrium systems. In the particular case of vanishing Γ , the SDE (2.4) reduces to the ODE

$$\dot{x}^i = \Pi^{ij}\partial_j H_t(x) + G_t^i(x) \quad (2.6)$$

describing a deterministic Hamiltonian dynamics in the presence of an additional force G_t .

Example 4. Langevin-Kramers equation. This is a special case of the Langevin dynamics that takes place in the phase space of n degrees of freedom with $x = (q, p)$ and

$$\Gamma = \begin{pmatrix} 0 & 0 \\ 0 & \gamma \end{pmatrix}, \quad \Pi = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad H_t = \frac{1}{2} p \cdot m^{-1} p + V_t(q), \quad G_t = (0, f_t(q)),$$

where $\gamma \neq 0$ is a non-negative $n \times n$ matrix, m^{-1} a positive one, and 1 the unit one. Here, Eq. (2.4) reduces to the standard relation $p_i = m_{ij}\dot{q}^j$ between momenta and velocities, where m is the mass matrix, and to the second order SDE,

$$m_{ij}\ddot{q}^j = -\gamma_{ik}\dot{q}^k - \partial_i V_t(q) + f_{ti}(q) + \zeta_i, \quad (2.7)$$

that we shall call Langevin-Kramers equation, with the n -dimensional white noise ζ such that

$$\langle \zeta_{it} \zeta_{jt'} \rangle = 2\beta^{-1} \gamma_{ij} \delta(t-t').$$

The Langevin-Kramers equation has the form of the Newton equation with the friction $-\gamma\dot{q}$ and white-noise ζ_t forces supplementing the conservative one $-\nabla V_t$ and the additional one f_t . It was discussed in [57] in a very similar context. In the limit of a strongly overdamped system when the friction term becomes much larger than the second order one, the Langevin-Kramers equation (2.7) reduces to the first order SDE,

$$\gamma_{ik}\dot{q}^k = -\partial_i V_t(q) + f_{ti}(q) + \zeta_i,$$

which, if $\gamma > 0$, may be cast again into the form (2.4) but with $\Gamma = \gamma^{-1}$, $\Pi = 0$ and $H_t = V_t$. One should keep in mind this change when applying the results described below for the Langevin dynamics (2.4) to the overdamped Langevin-Kramers dynamics.

3. Transition Probabilities and Detailed Balance

Let us recall some basic facts about the diffusion processes in order to set the notations. We shall denote by $E_x^{t_0}$ the expectation of functionals of the Markov process \mathbf{x}_t solving the SDE (2.1) with the initial condition $\mathbf{x}_{t_0} = x$. For $t \geq t_0$, the relation

$$E_x^{t_0} g(\mathbf{x}_t) = \int P_{t_0,t}(x, dy) g(y) \equiv (P_{t_0,t}g)(x) \quad (3.1)$$

defines the transition probabilities $P_{t_0,t}(x, dy)$ of the process \mathbf{x}_t and the operator $P_{t_0,t}$. The transition probabilities satisfy the normalization condition $\int P_{t_0,t}(x, dy) = 1$ and the Chapman-Kolmogorov chain rule

$$\int P_{t_0,t}(x, dy) P_{t,t'}(y, dz) = P_{t_0,t'}(x, dz).$$

The evolution of the expectation values is governed by the second-order differential operators L_t defined by the relation

$$\frac{d}{dt} E_x^{t_0} g(\mathbf{x}_t) = E_x^{t_0} (L_t g)(\mathbf{x}_t). \quad (3.2)$$

The explicit form of L_t is found by a standard argument that involves the passage from the Stratonovich to the Itô convention. For reader's convenience, we give the details in Appendix A. The result is:

$$L_t = \hat{u}_t^i \partial_i + \frac{1}{2} \partial_j d_t^{ij} \partial_i, \quad (3.3)$$

where

$$d_t^{ij}(x) = D_t^{ij}(x, x) \quad \text{and} \quad \hat{u}_t^i(x) = u_t^i(x) - \frac{1}{2} \partial_{y^j} D_t^{ij}(x, y)|_{y=x}. \quad (3.4)$$

Due to the relation (3.1), Eq.(3.2) may be rewritten as the operator identity $\partial_t P_{t_0,t} = P_{t_0,t} L_t$. Together with the initial condition $P_{t_0,t_0} = 1$, it implies that $P_{t_0,t}$ is given by the time-ordered exponential

$$P_{t_0,t} = \overrightarrow{T} \exp \left(\int_{t_0}^t L_s ds \right) = \sum_{n=0}^{\infty} \int_{t_0 \leq s_1 \leq s_2 \leq \dots \leq s_n} L_{s_1} L_{s_2} \dots L_{s_n} ds_1 ds_2 \dots ds_n. \quad (3.5)$$

In particular, $P_{t_0,t} = e^{(t-t_0)L} \equiv P_{t-t_0}$ in the stationary case with $u_t \equiv u$ and $D_t \equiv D$. The operator $L_t \equiv L$ is then called the **generator** of the process.

The stochastic process \mathbf{x}_t may be used to evolve measures. Under the stochastic dynamics, the initial measure $\mu_{t_0}(dx)$ evolves at time t to the measure

$$\mu_t(dy) = \int \mu_{t_0}(dx) P_{t_0,t}(x, dy). \quad (3.6)$$

We shall use below the shorthand notation: $\mu_t = \mu_0 P_{0,t}$. For measures with densities $\mu_t(dx) = \rho_t(x) dx$ with respect to the Lebesgue measure dx , Eq.(3.6) is equivalent to the evolution equation

$$\partial_t \rho_t = \partial_i \left(-\hat{u}_t^i + \frac{1}{2} d_t^{ij} \partial_j \right) \rho_t \equiv L_t^\dagger \rho_t, \quad (3.7)$$

where L_t^\dagger is the (formal) adjoint of the operator L_t . The latter relation may be rewritten as the continuity equation

$$\partial_t \rho_t + \nabla \cdot j = 0 \quad \text{with} \quad j_t^i = (\hat{u}_t^i - \frac{1}{2} d_t^{ij} \partial_j) \rho_t, \quad (3.8)$$

where $\nabla \cdot j \equiv \partial_i j_t^i$ is the divergence of the **density current** j_t corresponding to the measure μ_t (the probability current, if μ_t is normalized). In the case with no explicit time dependence when $L_t \equiv L$, an invariant density ρ , corresponding to an invariant measure $\mu(dx) = \rho(x) dx$ of the process, satisfies the equation $L^\dagger \rho = 0$ which may be rewritten in the form of the current conservation condition $\nabla \cdot j = 0$. We shall often write the invariant density $\rho(x)$ in the exponential form as $e^{-\varphi(x)}$. One says that the process satisfies the **detailed balance relation** with respect to φ if the density current j related to the measure $\mu(dx) = e^{-\varphi(x)} dx$ vanishes itself, i.e. if

$$\hat{u}^i = -\frac{1}{2} d^{ij} \partial_j \varphi.$$

Equivalently, this condition may be written as the relation

$$L^\dagger = e^{-\varphi} L e^{\varphi},$$

for the generator of the process or as the identity

$$\mu(dx) P_t(x, dy) = \mu(dy) P_t(y, dx) \quad (3.9)$$

for the transition probabilities. In all these three forms, it implies directly that μ is an invariant measure. The converse, however, is not true: there exist stationary diffusion processes with invariant measures that do not satisfy the detailed balance relation.

The generator of the stationary Langevin equation with $\Pi = 0$ and $G = 0$ satisfies the detailed balance relation with respect to $\varphi = \beta H$ so that the Gibbs density $\rho(x) = e^{-\beta H(x)}$, and, if the latter is normalizable, the Gibbs probability measure $\mu^G(dx) = Z^{-1} e^{-\beta H(x)} dx$, are invariant under such dynamics. The invariance still holds when $\Pi \neq 0$ but, in this case, the detailed balance relation fails. We shall see below how to generalize the latter to catch also the case with conservative forces when $\Pi \neq 0$.

4. Tangent Process and Phase-Space Contraction

One may generate other processes of a similar nature from the diffusive process (2.1). Such constructions will play an important role in studying fluctuation relations. As the first example, let us consider the separation $\delta \mathbf{x}_t$ between the solution \mathbf{x}_t of Eq. (2.1) with the initial value $\mathbf{x}_0 = x$ and another solution infinitesimally close to \mathbf{x}_t . Such a separation evolves according to the law

$$\delta \mathbf{x}_t = \mathbf{X}_t(x) \delta \mathbf{x}_0,$$

where the matrix $\mathbf{X}_t(x)$ with the entries

$$X_{t,j}^i(x) = \frac{\partial x_t^i}{\partial x_0^j}(x) \quad (4.1)$$

solves the (Stratonovich) SDE

$$\dot{X}_{t,j}^i = (\partial_k u_t^i + \partial_k v_t^i)(\mathbf{x}_t) X_{t,j}^k \quad (4.2)$$

with the initial condition $X_0(x) = 1$. Together with Eq. (2.1), the SDE (4.2) defines a diffusion process $(\mathbf{x}_t, \mathbf{X}_t)$ that we shall call the **tangent process**. In particular, the quantity $-\ln \det \mathbf{X}_t$ that represents the accumulated phase-space contraction along the trajectory \mathbf{x}_t , solves the SDE

$$\frac{d}{dt}(-\ln \det X) = -(\nabla \cdot u_t + \nabla \cdot v_t)(\mathbf{x}_t). \quad (4.3)$$

The right hand side of Eq. (4.3) is the **phase-space contraction rate**. We infer that

$$-\ln \det \mathbf{X}_t = -\int_0^t (\nabla \cdot u_t)(\mathbf{x}_t) dt - \int_0^t (\nabla \cdot v_t)(\mathbf{x}_t) dt. \quad (4.4)$$

The second integral on the right hand side should be interpreted with the Stratonovich convention. The phase-space contraction is an important quantity in the study of nonequilibrium dynamics and it will reappear in the sequel.

5. Backward Processes

Among the diffusion processes that may be generated from the original process (2.1) are the ones which may be interpreted as its time reversals. The action of time inversion on space-time will be given by the transformation

$$(t, x) \longrightarrow (T - t, x^*) \equiv (t^*, x^*) \quad (5.1)$$

for an involution $x \mapsto x^*$. It may be lifted to the level of process trajectories by defining the transformed trajectory $\tilde{\mathbf{x}}_t$ by the relation

$$\tilde{\mathbf{x}}_t = \mathbf{x}_{t^*}^*. \quad (5.2)$$

In general, however, we shall **not** define the time-reversed process as $\tilde{\mathbf{x}}_t$ because, in the presence of dissipative deterministic forces like friction, such time inversion would lead to an anti-dissipative dynamics. We shall then allow for more flexibility. In order to define the time-reversed process, we shall divide the deterministic vector field u_t into two parts

$$u_t = u_{t,+} + u_{t,-}, \quad (5.3)$$

that we shall loosely term dissipative and conservative, choosing different time-inversion rules for them. The time-reversed process \mathbf{x}'_t will be given by the SDE

$$\dot{\mathbf{x}}' = u'_t(\mathbf{x}') + v'_t(\mathbf{x}') \quad (5.4)$$

with the deterministic vector field $u'_t = u'_{t,+} + u'_{t,-}$ and the random one v'_t defined by the equations

$$u'^i_{t,\pm}(x) = \pm(\partial_k x^{*i})(x^*) u^k_{t^*,\pm}(x^*) \quad \text{and} \quad v'^i_t(x) = \pm(\partial_k x^{*i})(x^*) v^k_{t^*}(x^*). \quad (5.5)$$

Note that $u_{t,+}$ transforms as a vector field under the involution $x \mapsto x^*$ and $u_{t,-}$ as a pseudo-vector field. For v_t we may use whichever rule since v_t and $-v_t$ have the same distribution. The SDE (5.4) for the time-reversed process \mathbf{x}'_t coincides with the one for the process $\tilde{\mathbf{x}}_t$ defined by Eq. (5.2) if and only if $u_{t,+}$ vanishes and v_t is transformed

according to the pseudo-vector rule. We shall call \mathbf{x}'_t the **backward process** referring to \mathbf{x}_t as the forward one. The random vector field v'_t of the backward process is again Gaussian with mean zero and white-noise behavior in time. Its covariance is

$$\langle v'_t{}^i(x) v'_s{}^j(y) \rangle = \delta(t-s) D_t{}^{ij}(x, y),$$

where

$$D_t{}^{ij}(x, y) = (\partial_k x^{*i})(x^*) D_t{}^{kl}(x^*, y^*) (\partial_l x^{*j})(y^*). \quad (5.6)$$

As before, see Eqs. (3.4), we shall denote

$$d_t{}^{ij}(x) = D_t{}^{ij}(x, x), \quad \hat{u}_t{}^i(x) = u_t{}^i(x) - \frac{1}{2} \partial_{y^j} D_t{}^{ij}(x, y)|_{y=x}. \quad (5.7)$$

Remark 1. Using the chain rule $(\partial_j x^{*i})(x^*)(\partial_k x^{*j})(x) = \delta_k^i$, it is easy to see that the time-inversion transformations (5.5) are involutive.

Let us emphasize that the choice of a time inversion consists of the choice of the involution (5.1) and of the splitting (5.3) of u_t . We shall call the process **time-reversible** (for a given choice of time inversion) if the deterministic vector fields u and u' of the forward and of the backward processes coincide and if the respective random vector fields v_t and v'_t have the same distribution, i.e. if

$$u_{t,+}^i(x) + u_{t,-}^i(x) = (\partial_k x^{*i})(x^*) (u_{t^*,+}^k(x^*) - u_{t^*, -}^k(x^*))$$

and if

$$D_t{}^{ij}(x, y) = (\partial_k x^{*i})(x^*) D_t{}^{kl}(x^*, y^*) (\partial_l x^{*j})(x^*). \quad (5.8)$$

Note that the first identity is equivalent to the relations

$$u_{t,\pm}^i(x) = \frac{1}{2} (u_t^i(x) \pm (\partial_k x^{*i})(x^*) u_{t^*}^k(x^*)) \quad (5.9)$$

and can be always achieved by taking such a splitting of u_t . It may be not easy, however, to realize physically the backward process corresponding to the splitting (5.9). The second condition (5.8) is a non-trivial constraint on the distribution of the white-noise velocity v_t . Nevertheless, if D_t is time-independent, it may be satisfied by choosing the trivial involution $x^* \equiv x$.

Parallely to the splitting (5.3) of the drifts u_t and u'_t , we shall divide the operators generating the forward and the backward evolution into two parts:

$$L_t = L_{t,+} + L_{t,-}, \quad L'_t = L'_{t,+} + L'_{t,-}$$

according to the formulae:

$$\begin{aligned} L_{t,+} &= \hat{u}_{t,+}^i \partial_i + \frac{1}{2} \partial_j d_t{}^{ij} \partial_i, & L_{t,-} &= u_{t,-}^i \partial_i, \\ L'_{t,+} &= \hat{u}_{t,+}^i \partial_i + \frac{1}{2} \partial_j d_t{}^{ij} \partial_i, & L'_{t,-} &= u_{t,-}^i \partial_i. \end{aligned}$$

The time-inversion rules become even more transparent when expressed in terms of the split generators. Let R denote the involution operator acting on the functions by

$$(Rf)(x) = f(x^*). \quad (5.10)$$

Lemma 1.

$$L'_{t,\pm} = \pm R L_{t^*,\pm} R. \quad (5.11)$$

Proof of Lemma 1, involving a straightforward although somewhat tedious check, is given in Appendix B.

Below, similarly as for the forward process, we shall denote by $E_x'^{t_0}$ the expectation of functionals of the backward process satisfying the initial condition $x'_{t_0} = x$. For $t \geq t_0$, the relations

$$E_x'^{t_0} g(x'_t) = (P'_{t_0,t} g)(x) \quad \text{with} \quad P'_{t_0,t} = \overrightarrow{T} \exp \left(\int_{t_0}^t L'_s ds \right)$$

define the operators whose kernels give the transition probabilities of the time-reversed process x'_t .

6. Examples of Time-Inversion Rules

The preceding considerations were very general. Physically, not all time-inversion rules for the diffusive processes (2.1) described above are on equal footing. In particular situations, some rules may be more natural or easier to implement than other ones. Let us list here a few cases of special time inversions that were discussed in the literature and/or will be used below.

6.1. Natural time inversion. Taking the trivial splitting $u_{t,+} = 0$, $u_{t,-} = u_t$ combined with an involution $x \mapsto x^*$ leads to the time-inversion rules that produce the backward process with trajectories related by the transformation (5.2) to the ones of the forward process if the pseudo-vector field rule is used when transforming v_t . This is the time inversion usually employed for the deterministic systems but it may be used more generally.

6.2. Time inversion with $\hat{u}_{t,+} = 0$. Consider the time inversion corresponding to an arbitrary involution $x \mapsto x^*$ and the choice

$$\hat{u}_{t,+} = 0, \quad u_{t,-} = \hat{u}_t. \quad (6.1)$$

of the splitting of u_t . Such a time inversion is a slight modification of the natural one to which it reduces in the case of deterministic dynamics (2.3) with $v_t \equiv 0$. As we show in Appendix C, the backward dynamics corresponding to the splitting (6.1) is given by the relations

$$\hat{u}_{t,+}^i(x) = \frac{1}{2} d_t^{ij}(x) (\partial_j \ln \sigma)(x), \quad u_{t,-}^i(x) = -(\partial_k x^{*i})(x^*) \hat{u}_{t^*}^k(x^*), \quad (6.2)$$

where $\sigma(x) = \sigma(x^*)^{-1}$ denotes the absolute value $|\det(\partial_j x^{*i})(x)|$ of the Jacobian of the involution $x \mapsto x^*$. The time inversion considered here will be used to obtain fluctuation relations in the limiting case of deterministic dynamics (2.3) when D_t^{ij} is set to zero and the backward dynamics is given by the ODE

$$\dot{x}^i = u_t^i(x') \quad \text{for} \quad u_t^i(x) = -(\partial_k x^{*i})(x^*) u_{t^*}^k(x^*), \quad (6.3)$$

obtained from the ODE (2.3) by the natural time inversion.

6.3. Time inversion in the Langevin dynamics. To explain why the rules of time inversion with non-vanishing $u_{t,+}$ are more generally needed, we consider the case of the Langevin dynamics that involves the dissipative force $-\Gamma \nabla H_t$. Let us arbitrarily split the corresponding drift u_t into two parts:

$$u_t = -\Gamma \nabla H_t + \Pi \nabla H_t + G_t = u_{t,+} + u_{t,-}, \quad (6.4)$$

see Eq. (2.4). Recall the relation (2.5) that aligns the matrix Γ with the covariance of the white-noise $v_t = \zeta_t$. It is natural to require the backward dynamics to be also of the Langevin type but for the time-reversed Hamiltonian $H'_t(x) = H_t^*(x^*)$. This requires that

$$u'_t = -\Gamma' \nabla H'_t + \Pi' \nabla H'_t + G'_t = u'_{t,+} + u'_{t,-}, \quad (6.5)$$

and that $v'_t(x) = \zeta'_t$ with the covariance of the white noise ζ'_t aligned with matrix Γ' as in Eq. (2.5). Upon restriction to linear involutions $x^* = rx$ with the matrix r squaring to 1, the transformation rules (5.5) become

$$u'_{t,\pm}(x) = \pm r u_{t^*,\pm}(rx), \quad \zeta'_t = \pm r \zeta_{t^*}.$$

The condition on the covariance of ζ'_t imposes the relation $\Gamma' = r \Gamma r^T$. Applying r to both sides of Eq. (6.5) taken at time t^* and at point rx , we infer that

$$-r \Gamma' r^T \nabla H_t(x) + r \Pi' r^T \nabla H_t(x) + r G'_{t^*}(rx) = u_{t,+}(x) - u_{t,-}(x).$$

The latter identity, together with Eq. (6.4), result in the relations

$$\begin{aligned} u_{t,+}(x) &= -\Gamma \nabla H_t(x) + \frac{1}{2}(\Pi + r \Pi' r^T) \nabla H_t(x) + \frac{1}{2}(G_t(x) + r G'_{t^*}(rx)), \\ u_{t,-}(x) &= -\frac{1}{2}(\Pi - r \Pi' r^T) \nabla H_t(x) + \frac{1}{2}(G_t(x) - r G'_{t^*}(rx)). \end{aligned}$$

At least when Γ is strictly positive, H_t is not a constant, and the extra force G_t is absent, one infers that the component $u_{t,+}$ cannot vanish identically by considering the contraction $(\nabla H_t) \cdot u_{t,+}$. We shall call **canonical** a choice of the time inversion for the Langevin dynamics for which

$$\Gamma' = r \Gamma r^T = \Gamma, \quad \Pi' = -r \Pi r^T = \Pi, \quad (6.6)$$

$$u_{t,+} = -\Gamma \nabla H_t, \quad u_{t,-} = \Pi \nabla H_t + G_t. \quad (6.7)$$

Note that such a time inversion treats the force G_t as a part of $u_{t,-}$ even when this force is of the non-conservative type. The Langevin dynamics is time-reversible under a canonical time inversion if $H'_t = H_t$ and $G'_t = G_t$. For the Langevin-Kramers equation, the standard phase-space involution $(q, p)^* = r(q, p) = (q, -p)$ verifies Eqs. (6.6) and it leads to the particularly simple canonical time-inversion rules with

$$V'_t = V_{t^*}, \quad f'_t = f_{t^*}$$

and to the time-reversibility if $V_t = V_{t^*}$ and $f_t = f_{t^*}$.

6.4. *Reversed protocol.* The time inversion corresponding to the choice

$$u_{t,+} = u_t, \quad u_{t,-} = 0 \quad (6.8)$$

and the trivial involution $x^* \equiv x$ was termed in [10] a reversed protocol. It may be viewed as consisting of the inversion of the time-parametrization in the vector fields in the SDE (2.1), if the vector-field rule is used to reverse v_t . In the stationary case, where it results in time-reversibility, such a time inversion was employed already in [59]. Here, we shall admit also a possibility of a non-trivial involution $x \mapsto x^*$. The reversed protocol leads then to the backward process with

$$u_{t,+}^i = (\partial_k x^{*i})(x^*) u_{t*}^k(x^*), \quad u_{t,-}^i = 0, \quad v_t^i = (\partial_k x^{*i})(x^*) v_{t*}^k(x^*). \quad (6.9)$$

6.5. *Current reversal.* Suppose that $e^{-\varphi_t}$ are densities satisfying $L_t^\dagger e^{-\varphi_t} = 0$. Such densities would be preserved by the evolution if the generator of the process were frozen to L_t . The density current corresponding to $e^{-\varphi_t}$ has the form

$$j_t^i = \left(\hat{u}_t^i + \frac{1}{2} d_t^{ij} (\partial_j \varphi_t) \right) e^{-\varphi_t},$$

see Eq.(3.8). It is conserved due to the relation $L_t^\dagger e^{-\varphi_t} = 0$. The time inversion defined by the choice

$$\hat{u}_{t,+}^i = -\frac{1}{2} d_t^{ij} \partial_j \varphi_t, \quad u_{t,-}^i = \hat{u}_t^i + \frac{1}{2} d_t^{ij} \partial_j \varphi_t, \quad (6.10)$$

and an arbitrary involution $x \mapsto x^*$ leads, after an easy calculation using the results of Appendix C, to the backward process with

$$\begin{aligned} \hat{u}_{t,+}^i &= -\frac{1}{2} d_t^{ij} \partial_j \varphi_t', \quad u_{t,-}^i(x) = -(\partial_k x^{*i})(x^*) u_{t*,-}^k(x^*) \\ v_t^i &= \pm (\partial_k x^{*i})(x^*) v_{t*}^i(x^*) \end{aligned} \quad (6.11)$$

for $\varphi_t'(x) = (\varphi_{t*} + \ln \sigma)(x^*)$. The density current for the backward process corresponding to the densities $e^{-\varphi_t'}$ is

$$\begin{aligned} j_t^i &= \left(\hat{u}_t^i + \frac{1}{2} d_t^{ij} (\partial_j \varphi_t') \right) e^{-\varphi_t'} \\ &= u_{t,-}^i(x) e^{-\varphi_t'(x)} = -(\partial_k x^{*i})(x^*) u_{t*,-}^k(x^*) e^{-\varphi_{t*}(x^*)} \sigma(x) \\ &= -(\partial_k x^{*i})(x^*) \left(\hat{u}_{t*}^k(x^*) + \frac{1}{2} d_{t*}^{kj}(x^*) (\partial_j \varphi_{t*})(x^*) \right) e^{-\varphi_{t*}} \sigma(x) \\ &= -(\partial_k x^{*i})(x^*) j^k(x^*) \sigma(x) \end{aligned} \quad (6.12)$$

and is also conserved, as is easy to check. It follows that $L_t^{\dagger'} e^{-\varphi_t'} = 0$. We shall term the time inversion corresponding to the choices (6.10) the **current reversal**. For $x^* \equiv x$ when it just reverses the sign of the density current, it was already employed in an implicit way in [43], and was introduced explicitly (under a different name) in [10]. The latter reference discussed also a simple two-dimensional model for which the inverse protocol and the current reversal led to different backward processes.

6.6. Complete reversal. Finally, modifying slightly the last scheme, let us suppose the densities $\rho_t = e^{-\varphi_t}$ evolve under the dynamics solving Eq. (3.7). With the same splitting (6.10) as for the current reversal, we obtain the backward process for which Eqs. (6.11) and (6.12) still hold for $\varphi'_t(x) = (\varphi_t^* + \ln \sigma)(x^*)$. We shall call the corresponding time inversion the **complete reversal**. Unlike in the other examples, it depends also on the choice of the initial density ρ_0 and may be difficult to realize physically. The time-reflected densities $\rho'_t = e^{-\varphi'_t}$ evolve now according to the backward-process version of Eq. (3.7). The current reversal and the complete reversal coincide in the case without explicit time dependence and with the choice of $\varphi_t \equiv \varphi$ such that $e^{-\varphi} dx$ is an invariant measure.

7. Relation Between Forward and Backward Processes

A comparison between the forward and the backward processes will be at the core of fluctuation relations that we shall discuss. To put the processes in the two time directions back-to-back, we shall adapt to the present setup the arguments developed in Sect. 5 of [59]. Let us introduce a perturbed version of the generator L_t of the forward process,

$$L_t^1 = L_t - 2\hat{u}_{t,+}^i \partial_i - (\partial_i \hat{u}_{t,+}^i) + (\partial_i u_{t,-}^i). \quad (7.1)$$

Operator L_t^1 is related in a simple way to the generator of the backward process:

$$\begin{aligned} R(L_t^1)^\dagger R &= R(\partial_i \hat{u}_{t,+}^i - \partial_i u_{t,-}^i + \frac{1}{2} \partial_i d_t^{ij} \partial_j - (\partial_i \hat{u}_{t,+}^i) + (\partial_i u_{t,-}^i)) R \\ &= R L_{t,+} - R L_{t,-} R = L_{t^*}^{\prime}, \end{aligned} \quad (7.2)$$

where R is defined by Eq. (5.10) and the last equality is a consequence of the relations (5.11). Let us consider the time-ordered exponential of the integral of L_t^1 . Using the relation $L_t^1 = (R L_{t^*}^{\prime} R)^\dagger$ that follows from Eq. (7.2), we infer that

$$\begin{aligned} P_{t_0,t}^1 &\equiv \overrightarrow{\mathcal{T}} \exp \left(\int_{t_0}^t L_s^1 ds \right) = \overleftarrow{\mathcal{T}} \exp \left(\int_{t^*}^{t_0^*} (R L_s^{\prime} R)^\dagger ds \right) \\ &= \left[R \overrightarrow{\mathcal{T}} \exp \left(\int_{t^*}^{t_0^*} L_s^{\prime} ds \right) R \right]^\dagger = (R P_{t^*,t_0^*}^{\prime} R)^\dagger. \end{aligned} \quad (7.3)$$

Above, the first inversion of the time order from $\overrightarrow{\mathcal{T}}$ to $\overleftarrow{\mathcal{T}}$ was due to the change of integration variables $s \mapsto s^* = T - s$, and the second one, to the fact that the hermitian conjugation reverses the order in the product of operators. Let us remark that $\frac{A(y,dx)}{dx} dy$ is the kernel of the operator A^\dagger and $A(x^*, dy^*)$ of the operator $R A R$ if $A(x, dy)$ is the kernel of a real operator A . Rewriting Eq. (7.3) in terms of the kernels, with these comments in mind, we obtain the identity

$$dx P_{t_0,t}^1(x, dy) = dy P_{t^*,t_0^*}^{\prime}(y^*, dx^*). \quad (7.4)$$

Remark 2. The transition probability of the backward process on the right hand side may be replaced by the one of the forward process in the time-reversible case.

Note that the 2nd order differential operator L_t^1 differs from L_t only by lower order terms, see Eq. (7.1). A combination of the Cameron-Martin-Girsanov and the Feynman-Kac formulae [79] permits to express the kernel $P_{t_0,t}^1(x, dy)$ as a perturbed expectation for the forward process.

Lemma 2. *If the matrix $(d_t^{ij}(x))$ is invertible for all t and x then*

$$P_{t_0,t}^1(x, dy) = E_x^{t_0} e^{-\int_{t_0}^t \mathcal{J}_s ds} \delta(\mathbf{x}_t - y) dy, \quad (7.5)$$

where

$$\mathcal{J}_t = 2 \hat{u}_{t,+}(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t) \dot{\mathbf{x}}_t - 2 \hat{u}_{t,+}(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t) u_{t,-}(\mathbf{x}_t) - (\nabla \cdot u_{t,-})(\mathbf{x}_t) \quad (7.6)$$

is a (local) functional of the solution \mathbf{x}_t of the SDE (2.1). The right hand side of Eq. (7.6) uses the vector notation. The first term in the expression for \mathcal{J}_t has to be interpreted with the Stratonovich convention.

Proof of Lemma 2 is deferred to Appendix D. A combination of the relations (7.5) and (7.4) gives immediately

Proposition 1.

$$dx E_x^{t_0} e^{-\int_{t_0}^t \mathcal{J}_s ds} \delta(\mathbf{x}_t - y) dy = dy P_{t^*,t_0^*}'(y^*, dx^*). \quad (7.7)$$

This is the first fluctuation relation of a series to be considered. It connects the transition probability of the backward process to an expectation in the forward process weighted with an exponential factor. Let us illustrate this relation in a few particular situations related to the examples of the diffusion processes considered in Sect. 2.

Example 5. Tangent process in the stationary homogeneous Kraichnan model. Recall Sect. 4 devoted to the definition of a tangent process. Let us consider the tangent process $(\mathbf{x}_t, \mathbf{X}_t)$ with fixed initial data $\mathbf{x}_0 = x$ and $\mathbf{X}_0 = 1$ for the homogeneous Kraichnan model. As was discussed in detail in [40], in this case, the distribution of the process \mathbf{X}_t may be obtained by solving, instead of the SDE (4.2) with $u_t \equiv 0$, a simpler linear Itô SDE

$$dX = S_t dt X \quad (7.8)$$

with a matrix-valued white-noise S_t such that

$$\langle S_{tk}^i S_{sl}^j \rangle = -\delta(t-s) \partial_k \partial_l D^{ij}(0).$$

In other words, in Eq. (4.2), we may replace $\partial_k v^i(\mathbf{x}_t)$ by $\partial_k v_t^i(0) \equiv S_{tk}^i$, if we change the SDE convention to the Itô one at the same time. Consequently, in the homogeneous Kraichnan model, the process \mathbf{X}_t may be decoupled from the original process \mathbf{x}_t . Let

us abbreviate: $-\partial_k \partial_l D_t^{ij}(0) = C_{kl}^{ij}$. Remark the symmetries $C_{kl}^{ij} = C_{lk}^{ji} = C_{lk}^{ij} = C_{kl}^{ji}$. The Itô SDE (7.8) may be rewritten as the equation

$$\dot{X}_j^i = -\frac{1}{2} C_{kl}^{ik} X_j^l + S_{tl}^i X_j^l \quad (7.9)$$

that employs the Stratonovich convention. Upon the use of the notations:

$$U_j^i(X) = -\frac{1}{2} C_{kl}^{ik} X_j^l, \quad V_{tj}^i(X) = S_{tl}^i X_j^l,$$

it may be cast into the form

$$\dot{X} = U(X) + V_t(X), \quad (7.10)$$

falling within the scope of (stationary) diffusion SDEs (2.1) and defining a Markov process X_t . The covariance of the white-noise “velocity” $V_t(X)$ is

$$\left\langle V_{tk}^i(X) V_{sl}^j(Y) \right\rangle = \delta(t-s) D_{kl}^{ij}(X, Y) \quad \text{with} \quad D_{kl}^{ij}(X, Y) = C_{nm}^{ij} X_k^n Y_l^m.$$

As in the general case (3.4), we shall denote:

$$d_{kl}^{ij}(X) = D_{kl}^{ij}(X, X) \quad \hat{U}_j^i(X) = U_j^i(X) - \frac{1}{2} \partial_{\tilde{X}_l^k} D_{jl}^{ik}(X, Y)|_{Y=X} = -\frac{d+1}{2} C_{nk}^{ni} X_j^k.$$

Let us apply the reversed-protocol time inversion discussed in Sect. 6.4 to the forward SDE (7.10). It corresponds to the trivial splitting of U with $U_+ = U$ and $U_- = 0$ and to an involution $X \mapsto X^*$ that we shall also take trivial: $X^* \equiv X$. The backward evolution is then given by the same equation (7.9) with S_t replaced by $S_t' = S_t^*$, a matrix-valued white noise with the same distribution as S_t . The time-reversibility follows. Suppose that the covariance C of the white noise $S(t)$ is invertible³, i.e. that there exists a matrix $(C^{-1})_{jm}^{ln}$ such that $C_{kl}^{ij} (C^{-1})_{jm}^{ln} = \delta_m^i \delta_k^n$. Then the matrix

$$(d^{-1})_{jm}^{ln}(X) = (X^{-1})_p^l (X^{-1})_r^n (C^{-1})_{jm}^{pr}$$

provides the inverse of $d_{kl}^{ij}(X)$. Substituting these data into Eq. (7.6), we obtain

$$\mathcal{J}_t = 2(\hat{U})_l^j(X_t) (d^{-1})_{jm}^{ln}(X_t) \dot{X}_{tn}^m = -(d+1) (X_t^{-1})_m^n \dot{X}_{tn}^m = -(d+1) \frac{d}{dt} \ln |\det X_t|.$$

The relation (7.7) applied to the case at hand leads to the identity

$$dX_0 P_t(X_0, dX) |\det X_0|^{-(d+1)} |\det X|^{d+1} = dX P_t(X, dX_0), \quad (7.11)$$

where $P_t(X_0, dX)$ denotes the transition probability of the forward process X_t solving the SDEs (7.8) or (7.9) and dX_0 on the left hand side and dX on the right hand side stand for the Lebesgue measures on the space of $d \times d$ matrices. We made use of the fact that the backward process has the same law as the forward one. Equation (7.11) is nothing else but the detailed balance relation with respect to $\varphi(X) = (d+1) \ln |\det X|$.

³ The assumption about invertibility of C may be dropped at the end by a limiting argument.

Indeed, note that the density current corresponding to the density $\rho(X) = |\det X|^{-d+1}$

$$j(X) = \left(\hat{U}(X) + \frac{1}{2} d(X) \nabla \varphi \right) |\det X|^{-d+1},$$

see Eq. (3.8), vanishes.

Integrating the left hand side of the identity (7.11) against a function $f(X_0, X)$ and using the relation $P_t(X_0, dX) = P_t(1, d(XX_0^{-1}))$ that follows from the invariance of the corresponding SDE under the right multiplication of X by invertible matrices, we obtain the equalities

$$\begin{aligned} & \int f(X_0, X) \det(XX_0^{-1})^{d+1} dX_0 P_t(X_0, dX) \\ &= \int f(X_0, X) \det(XX_0^{-1})^{d+1} dX_0 P_t(1, d(XX_0^{-1})) \\ &= \int f(X_0, XX_0) (\det X)^{d+1} dX_0 P_t(1, dX) \\ &= \int f(X^{-1}X_0, X_0) (\det X) dX_0 P_t(1, dX), \end{aligned}$$

where we twice changed variables in the iterated integrals. On the other hand, the integration of the right hand side of Eq. (7.11) against $f(X_0, X)$ gives

$$\begin{aligned} \int f(X_0, X) dX P_t(X, dX_0) &= \int f(X, X_0) dX_0 P_t(X_0, dX) \\ &= \int f(XX_0, X_0) dX_0 P_t(1, dX) \\ &= \int f(X^{-1}X_0, X_0) dX_0 P_t(1, dX^{-1}). \end{aligned}$$

Comparing the two expressions, we infer that

$$P_t(1, dX) (\det X) = P_t(1, dX^{-1}). \quad (7.12)$$

This is a version of the Evans-Searles [25] fluctuation relation for the stationary homogeneous Kraichnan model. In the context of general hydrodynamic flows, it was formulated and proven by a change-of-integration-variables argument in [1], see also [40]. We shall return in Sect. 15 to the relation (7.12) in order to examine some of its consequences. Subsequently, we shall generalize it in Sect. 16 to arbitrary diffusion processes of the type (2.1).

Example 6. Generalized detailed balance relation. Consider the complete-reversal rules discussed in Sect. 6.6 and corresponding to the choice (6.10). Since, by virtue of the assumption that the densities $e^{-\varphi_t}$ evolve under the dynamics, see Eq. (3.7),

$$L_t^\dagger e^{-\varphi_t} = -\partial_i u_{t,-}^i e^{-\varphi_t} = e^{-\varphi_t} (u_{t,-}^i \partial_i \varphi_t - \partial_i u_{t,-}^i) = -e^{-\varphi_t} \partial_t \varphi_t, \quad (7.13)$$

the last two terms in the definition (7.6) reduce to $-(\partial_t \varphi_t)(\mathbf{x}_t)$ in this case so that

$$\mathcal{J}_t = -(\nabla \varphi_t)(\mathbf{x}_t) \cdot \dot{\mathbf{x}}_t - (\partial_t \varphi_t)(\mathbf{x}_t) = -\frac{d}{dt} \varphi_t(\mathbf{x}_t). \quad (7.14)$$

Upon integration over time, this produces boundary terms and Eq.(7.7) implies the **generalized detailed balance relation**:

$$\mu_0(dx) P_{0,T}(x, dy) = \mu_T(dy) P'_{0,T}(y^*, dx^*), \quad (7.15)$$

for $\mu_t(dx) = e^{-\varphi_t(x)} dx$. Note that Eq.(7.15) holds for any choice of the involution $x \mapsto x^*$. Upon integration over x , it assures that the measures μ_t stay invariant under the dynamics, what was assumed from the very beginning. In the case with no explicit time dependence, i.e. when $L_t \equiv L$, Eq.(7.15) holds, in particular, for $\varphi_t \equiv \varphi$ such that $\mu = e^{-\varphi} dx$ is an invariant measure. In that case, the generalized detailed balance relation reduces to the detailed balance one (3.9) if u_- in the splitting (6.10) vanishes and $x^* \equiv x$. This was the case in Example 5. Below, we shall see examples where the invariant measure μ is known and the generalized detailed balance relation holds but where the detailed balance itself fails. Some of those cases fall under the scope of the Langevin dynamics. Let us discuss them first.

Example 7. 1st law of thermodynamics and generalized detailed balance for Langevin dynamics. For Langevin dynamics with the splitting (6.7) of the drift, a direct substitution yields

$$\mathcal{J}_t = -\beta(\nabla H_t)(\mathbf{x}_t) \cdot \dot{\mathbf{x}}_t + \beta(\nabla H)(\mathbf{x}_t) \cdot G_t(\mathbf{x}_t) - (\nabla \cdot G_t)(\mathbf{x}_t) \equiv \mathcal{J}_t^{Lan}.$$

Upon the use of the dynamical equation (2.4),

$$\begin{aligned} \int_0^T \mathcal{J}_t^{Lan} dt &= \int_0^T [\beta(\nabla H_t)(\mathbf{x}_t) \cdot \Gamma(\nabla H_t)(\mathbf{x}_t) - \beta(\nabla H_t)(\mathbf{x}_t) \cdot \zeta_t \\ &\quad - (\nabla \cdot G_t)(\mathbf{x}_t)] dt \equiv \beta Q, \end{aligned} \quad (7.16)$$

where Q may be identified with the heat transferred to the environment modeled by the thermal noise. On the other hand, using the original expression for \mathcal{J}_t^{Lan} together with the (Stranovich convention) identity $\frac{d}{dt} H_t(\mathbf{x}_t) = (\nabla H_t)(\mathbf{x}_t) \cdot \dot{\mathbf{x}}_t + (\partial_t H_t)(\mathbf{x}_t)$, we obtain the relation

$$\int_0^T \mathcal{J}_t^{Lan} dt = -\beta \Delta U + \beta W, \quad (7.17)$$

where $\Delta U = H_T(\mathbf{x}_T) - H_0(\mathbf{x}_0)$ is the change of the internal energy of the system and

$$W = \int_0^T [(\partial_t H_t)(\mathbf{x}_t) + (\nabla H)(\mathbf{x}_t) \cdot G_t(\mathbf{x}_t) - \beta^{-1}(\nabla \cdot G_t)(\mathbf{x}_t)] dt \quad (7.18)$$

may be interpreted as the work performed on the system. With these interpretations, a comparison of the two expressions for the integral of \mathcal{J}_t^{Lan} leads to the **1st law of thermodynamics**:

$$\Delta U = -Q + W. \quad (7.19)$$

This was discussed in a simple example of the forced and damped oscillator in [53]. In the absence of the extra force G_t , the expression for the work reduces to

$$W = \int_0^T (\partial_t H_t)(\mathbf{x}_t) dt \quad (7.20)$$

and represents the so called **Jarzynski work** introduced in [48] for deterministic Hamiltonian dynamics. In the stochastic Langevin-Kramers dynamics, the expressions for the heat and the work become:

$$Q = \int_0^T [\dot{q}_t \cdot \gamma \dot{q}_t - \dot{q}_t \cdot \zeta_t] dt, \quad W = \int_0^T [(\partial_t V_t)(q_t) + \dot{q}_t \cdot f_t(q_t)] dt. \quad (7.21)$$

The second quantity is equal to the sum of the Jarzynski work and of the work of the external force f_t . It was introduced and discussed in [57]. In the stationary case, it reduces to the injected work [56] and, up to the β -factor, coincides with the “action functional” (for uniform temperature) given by Eq. (6.3) of [59]. Note that the general expression (7.18) for work also makes sense in the case of deterministic dynamics (2.6) obtained from the SDE (2.4) by setting $\Gamma = 0$, in particular for the deterministic Hamiltonian evolution with $G_t \equiv 0$.

If $G_t \equiv 0$, the splitting (6.7) is a special case of the splitting used for the current reversal for $\varphi_t = \beta H_t$, see Eq. (6.10). In particular, if $H_t \equiv H$ then the transition probabilities of the Langevin process satisfy the generalized detailed balance relation (7.15) that takes the form

$$\mu(dx) P_T(x, dy) = \mu(dy) P'_T(y^*, dx^*) \quad (7.22)$$

for $\mu(dx) = e^{-\beta H(x)} dx$ and any involution $x \mapsto x^* = rx$. The latter identity replaces in the presence of the conservative force $\Pi \nabla H$ the detailed balance relation (3.9) and still assures that the Gibbs density $e^{-\beta H}$ is invariant under such Langevin dynamics. If the involution r satisfies additionally the relations (6.6) and $H(rx) = H(x)$, resulting in the time-reversibility, then one may replace P'_T by P_T in Eq. (7.15).

Example 8. Linear Langevin equation. Consider the linear SDE

$$\dot{x} = Mx + \zeta_t, \quad (7.23)$$

where M is a $d \times d$ matrix and ζ_t is the white noise with the covariance (2.5) and matrix Γ strictly positive. We shall be interested in cases when the matrix $\Gamma^{-1}M$ is non-symmetric. For an elementary discussion of mathematical aspects of such SDEs see e.g. [42]. In the context of nonequilibrium statistical mechanics, examples of such linear equations were considered in [58] as models of a harmonic chain of oscillators interacting with environment of variable temperature or, quite recently, in [81] for modeling coiled polymers in a shearing flow. The diffusion process \mathbf{x}_t that solves Eq. (7.23) with the initial value $\mathbf{x}_0 = x$ is given by the formula

$$\mathbf{x}_t = e^{tM} x + \int_0^t e^{(t-s)M} \zeta_s ds.$$

The transition probabilities of this process are Gaussian and have the explicit form

$$P_t(x, dy) = \det(2\pi\beta^{-1}C_t)^{-1/2} \exp\left[-\frac{\beta}{2}(y - e^{tM}x) \cdot C_t^{-1}(y - e^{tM}x)\right] dy, \quad (7.24)$$

where

$$C_t = 2 \int_0^t e^{sM} \Gamma e^{sM^T} ds \quad (7.25)$$

is a strictly positive matrix. Suppose that all the eigenvalues λ of M have negative real parts. Under this condition, e^{tM} tends to zero exponentially fast when $t \rightarrow \infty$ so that $C_\infty \equiv C$ is finite and

$$P_t(x, dy) \xrightarrow{t \rightarrow \infty} \det(2\pi\beta^{-1}C)^{-1/2} \exp\left[-\frac{\beta}{2}y \cdot C^{-1}y\right] dy,$$

with the right hand side defining the unique invariant probability measure of the process. This Gaussian measure has the form of the Gibbs measure for the quadratic Hamiltonian

$$H(x) = \frac{1}{2} x \cdot C^{-1} x. \quad (7.26)$$

Introducing the matrix

$$\Pi = \Gamma + MC \quad (7.27)$$

that is antisymmetric:

$$\begin{aligned} \Pi + \Pi^T &= 2\Gamma + 2 \int_0^\infty e^{sM} (M\Gamma + \Gamma M^T) e^{sM^T} ds \\ &= 2\Gamma + 2 \int_0^\infty \frac{d}{ds} e^{sM} \Gamma e^{sM^T} ds = 0, \end{aligned}$$

the linear SDE (7.23) may be rewritten in the Langevin form (2.4) as

$$\dot{x} = -\Gamma \nabla H(x) + \Pi \nabla H(x) + \zeta_t. \quad (7.28)$$

Conversely, the last SDE with H as in Eq.(7.26) for some $C > 0$ is turned into the form (7.23) upon setting

$$M = -(\Gamma - \Pi)C^{-1}. \quad (7.29)$$

Note that the last equation implies the relation (7.27) for Π . In Appendix E, we show that M given by Eq.(7.29) has necessarily all eigenvalues with negative real part and that C may be recovered from M as C_∞ given by Eq.(7.25) with $t = \infty$. This establishes the equivalence between the SDEs (7.23) and (7.28).

The probability current associated by the formula (3.8) to the Gaussian invariant Gibbs measure $\mu^G(dx) = Z^{-1}e^{-\beta H(x)}dx$ is

$$j(x) = Z^{-1}\Pi C^{-1}x e^{-\beta H(x)}.$$

It vanishes only when $\Pi = 0$. In the latter case, the transition probabilities (7.24) satisfy the detailed balance relation (3.9) for $\varphi = \beta H + \ln Z$. If $\Pi \neq 0$ then only a generalized detailed balance relation (7.22) holds for any choice of the linear involution $x \mapsto x^* = rx$. If moreover $r\Gamma r^T = \Gamma$, $r\Pi r^T = -\Pi$ and $rCr^T = C$, then P'_T on the right hand side of Eq. (7.15) may be replaced by P_T .

8. Jarzynski Equality

We shall exploit further consequences of the relation (7.7) between the forward and the backward processes. In this section we shall derive an identity that generalizes the celebrated Jarzynski equality [48, 49] and shall prepare the ground for obtaining more refined fluctuation relations following the ideas of [31, 63] and [19]. Let φ_0 and φ_T be two functions generating measures

$$\mu_0(dx) = e^{-\varphi_0(x)}dx, \quad \mu_T(dx) = e^{-\varphi_T(x)}dx, \quad (8.1)$$

respectively. In particular, we could take $e^{-\varphi_T(x)}$ such that the measure μ_T is related to μ_0 by the dynamical evolution (3.6), i.e. $\mu_T = \mu_0 P_{0,T}$, but we shall not assume such a choice unless explicitly stated. In general, the measures (8.1) may be not normalizable but we shall impose the normalization condition later on. We shall associate to μ_0 and μ_T the time-reflected measures

$$\mu'_0(dx) = e^{-\varphi'_0(x)}dx = e^{-\varphi_T(x^*)}dx^*, \quad \mu'_T(dx) = e^{-\varphi'_T(x)}dx = e^{-\varphi_0(x^*)}dx^*.$$

Let us modify the functional $\int_0^T \mathcal{J}_t dt$ introduced in the last section by boundary terms $\Delta\varphi \equiv \varphi_T(\mathbf{x}_T) - \varphi_0(\mathbf{x}_0)$ by setting

$$\mathcal{W} = \Delta\varphi + \int_0^T \mathcal{J}_t dt. \quad (8.2)$$

The functional \mathcal{W} will be the basic quantity in what follows. Its physical interpretation in terms of the entropy production will be discussed in Sect. 10 below.

For any functional \mathcal{F} on the space of trajectories \mathbf{x}_t parametrized by time in the interval $[0, T]$, we shall denote by $\tilde{\mathcal{F}}$ the functional defined by $\tilde{\mathcal{F}}(\mathbf{x}) = \mathcal{F}(\tilde{\mathbf{x}})$, where $\tilde{\mathbf{x}}$ is given by Eq. (5.2). We shall also introduce the shorthand notation

$$E_{x,y}^{0,T} \mathcal{F}(\mathbf{x}) = E_x^0 \mathcal{F}(\mathbf{x}) \delta(\mathbf{x}_T - y)$$

for the (unnormalized) expectation of the process \mathbf{x}_t with fixed initial and final points, and similarly for the backward process. The following refinement of the relation (7.7) of Proposition 1 holds:

Proposition 2.

$$\mu_0(dx) E_{x,y}^{0,T} \mathcal{F}(\mathbf{x}) e^{-\mathcal{W}(\mathbf{x})} dy = \mu'_0(dy^*) E_{y^*,x^*}^{0,T} \tilde{\mathcal{F}}(\mathbf{x}') dx^*. \quad (8.3)$$

Proof of Proposition 2 is contained in Appendix F. Note that the explicit dependence on the choice of measures μ_0 and μ'_0 trivially cancels the one buried in \mathcal{W} . In particular, for $\mathcal{F} \equiv 1$, Proposition 2 reduces to Proposition 1 with $t_0 = 0$ and $t = T$. As before, the backward-process expectation E' may be replaced by the forward-process one E for the time-reversible process.

If the measures μ_0 and μ'_0 are normalized then we may use them as the probability distributions of the initial points of the forward and of the backward process, respectively. The corresponding probability measures $M(d\mathbf{x})$ and $M'(d\mathbf{x}')$ on the space of trajectories on the time-interval $[0, T]$ are given by the relations

$$\int \mathcal{F}(\mathbf{x}) M(d\mathbf{x}) = \int \left(E_x^0 \mathcal{F}(\mathbf{x}) \right) \mu_0(dx) \equiv \langle \mathcal{F} \rangle, \quad (8.4)$$

$$\int \mathcal{F}(\mathbf{x}') M'(d\mathbf{x}') = \int \left(E_x^{0,T} \mathcal{F}(\mathbf{x}') \right) \mu'_0(dx) \equiv \langle \mathcal{F} \rangle'. \quad (8.5)$$

Upon integration over x and y , the identity (8.3) induces the following equality between the expectations with respect to the trajectory measures M and M' :

Corollary 1.

$$\langle \mathcal{F} e^{-\mathcal{W}} \rangle = \langle \tilde{\mathcal{F}} \rangle'. \quad (8.6)$$

It was stressed in [63], and even more explicitly in [19], that the identity of the type of (8.6), comparing the expectations in the forward and the backward processes, is a source of fluctuation relations. An important special case of Eq.(8.6) is obtained by setting $\mathcal{F} \equiv 1$. It was derived in [48] in the context of the Hamiltonian dynamics and in [49] in the one of Markov processes:

Corollary 2. (Jarzynski equality).

$$\langle e^{-\mathcal{W}} \rangle = 1. \quad (8.7)$$

Let us illustrate the meaning of the above relation by considering a few special cases.

Example 9. The case of Langevin dynamics. With the splitting (6.7) used for the canonical time inversion, upon taking $\varphi_t = \beta(H_t - F_t)$, where $F_t = -\beta^{-1} \ln \int e^{-\beta H_t(x)} dx$ denotes the free energy, we infer from Eq.(7.17) that

$$\mathcal{W} = \beta(\mathbf{W} - \Delta F), \quad (8.8)$$

where $\Delta F = F_T - F_0$ is the free energy change and \mathbf{W} is the work given by Eq.(7.18). The difference $\mathbf{W} - \Delta F$ is often called the **dissipative work**. The Jarzynski equality (8.7) may be rewritten in this case in the original form

$$\langle e^{-\beta \mathbf{W}} \rangle = e^{-\beta \Delta F}, \quad (8.9)$$

in which it has become a tool to compute the differences between free energies of equilibrium states from nonequilibrium processes [45, 17, 72, 73].

Example 10. The case of deterministic dynamics. Upon splitting the drift u_t with $\hat{u}_{t,+} \equiv 0$ related to the modified natural time inversion described in Sect. 6.2, the expression (7.6) reduces to

$$\mathcal{J}_t = -(\nabla \cdot \hat{u}_t)(\mathbf{x}_t) \equiv \widehat{\mathcal{J}_t^{nat}}. \quad (8.10)$$

For the deterministic dynamics where $D_t^{ij}(x, y) \equiv 0$, the difference between the vector fields \hat{u}_t and u_t disappears and $\widehat{\mathcal{J}_t^{nat}}$ reduces to

$$\mathcal{J}_t^{det} = -(\nabla \cdot u_t)(\mathbf{x}_t). \quad (8.11)$$

The right hand side represents the phase-space contraction rate along the trajectory \mathbf{x}_t , see Eq.(4.3). In this case,

$$\mathcal{W} = \Delta\varphi - \int_0^T (\nabla \cdot u_t)(\mathbf{x}_t) dt = \int_0^T \left[\frac{d}{dt} \varphi_t(\mathbf{x}_t) - (\nabla \cdot u_t)(\mathbf{x}_t) \right] dt \equiv \mathcal{W}^{det}. \quad (8.12)$$

For $\varphi_T = \varphi_0 = \varphi$, the last integral in Eq.(8.12) was termed “the integral of the **dissipation function**” in [26]. In the case of the deterministic dynamics (2.6) obtained from the Langevin equation by setting $\Gamma = 0$, the expression (8.12) for \mathcal{W} reduces to the one of Eq.(8.8) if we take $\varphi_t = \beta(H_t - F_t)$. In the deterministic case, the Jarzynski equality (8.7) reads

$$\int e^{\int_0^T (\nabla \cdot u_t)(\mathbf{x}_t) dt} e^{-\varphi_T(\mathbf{x}_T)} d\mathbf{x}_0 = 1 \quad (8.13)$$

and may be easily proven directly. To this end recall Eq.(4.4) which implies for the deterministic case that $\int_0^T (\nabla \cdot u_t)(\mathbf{x}_t) dt = \ln \det \mathbf{X}_T(\mathbf{x}_0)$, where the matrices $\mathbf{X}_t(x)$ of the tangent process are given by Eq.(4.1). The equality (8.13) is then obtained by the change of integration variables $\mathbf{x}_0 \mapsto \mathbf{x}_T$ whose Jacobian is equal to $\det \mathbf{X}_T(\mathbf{x}_0)$.

Example 11. The reversed protocol case. In the setup of Sect. 6.4 with $u_{t,-} = 0$,

$$\mathcal{J}_t = 2\hat{u}_t(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t) \dot{\mathbf{x}}_t \equiv \mathcal{J}_t^{tot}.$$

In the stationary case, the integral $\int_0^T \mathcal{J}_t^{tot} dt$, rewritten with use of the Itô convention, was termed an “action” in [59], see Eq.(5.3) therein. In [43], it was considered in the context of the Langevin equation with the extra force G_t (but without the Hamiltonian term $\Pi \nabla H_t$). It was then identified as $\beta \mathbf{Q}^{tot}$ with the quantity \mathbf{Q}^{tot} interpreted, following [68], as the **total heat** produced in the environment. The functional \mathcal{W} of the forward process is given here by the formula

$$\mathcal{W} = \Delta\varphi + 2 \int_0^T \hat{u}_t(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t) \dot{\mathbf{x}}_t dt \equiv \mathcal{W}^{tot}. \quad (8.14)$$

In particular, for the Langevin dynamics (2.4), one obtains:

$$\mathcal{W}^{tot} = \Delta\varphi + \beta \int_0^T (-\Gamma \nabla H_t + \Pi \nabla H_t + G_t)(\mathbf{x}_t) \cdot \Gamma^{-1} \dot{\mathbf{x}}_t dt. \quad (8.15)$$

The Jarzynski equality (8.7) was discussed for this case in [43, 78, 10]. Note that \mathcal{W}^{tot} is not well defined for the Langevin-Kramers dynamics. On the other hand, for the linear Langevin equation of Example 8 and for $\varphi_t = \beta(H - F)$,

$$\mathcal{W}^{tot} = \beta \int_0^T \mathbf{x}_t \cdot (C^{-1} + M^T \Gamma^{-1}) \dot{\mathbf{x}}_t dt = -\beta \int_0^T \mathbf{x}_t \cdot C^{-1} \Pi \Gamma^{-1} \dot{\mathbf{x}}_t dt \quad (8.16)$$

and it vanishes if $\Pi = 0$. A long time asymptotics of the probability distribution of a quantity differing from the last one by a boundary term was studied in [81].

Example 12. Hatano-Sasa equality [43]. In the current-reversal setup of Sect. 6.5, with the splitting (6.10) of the drift u_t induced by the normalized densities $e^{-\varphi_t}$ such that $L_t^\dagger e^{-\varphi_t} = 0$,

$$\mathcal{J}_t = -(\nabla \varphi_t)(\mathbf{x}_t) \cdot \dot{\mathbf{x}}_t \equiv \mathcal{J}_t^{ex}, \quad (8.17)$$

since now the last two terms on the right hand side of Eq.(7.6) vanish, compare to Eq.(7.13). Upon integration, this gives:

$$\int_0^T \mathcal{J}_t^{ex} dt = -\Delta\varphi + \int_0^T (\partial_t \varphi_t)(\mathbf{x}_t) dt. \quad (8.18)$$

In [43], the integral given by Eq.(8.17) was identified in the context of the Langevin equation with the force G_t as equal to $\beta \mathbf{Q}^{ex}$, where \mathbf{Q}^{ex} was termed the **excess heat**, following [68]. The difference $\mathbf{Q}^{tot} - \mathbf{Q}^{ex} = \mathbf{Q}^{hk}$ was called, in turn, the **housekeeping heat** and was interpreted as the heat production needed to keep the system in a nonequilibrium stationary state, see again [68, 43, 78, 10]. Using in the definition (8.2) the functions φ_0 and φ_T from the same family, we infer from Eq.(8.18) that

$$\mathcal{W} = \int_0^T (\partial_t \varphi_t)(\mathbf{x}_t) dt \equiv \mathcal{W}^{ex}. \quad (8.19)$$

The equality (8.7) for this case was proven by Hatano-Saso [43], see also [57]. Note that in the stationary case, $\mathcal{W}^{ex} = 0$. The Langevin dynamics discussed in Example 9 provides a special instance of the situation considered here if $G_t \equiv 0$. Consequently, in that case, \mathcal{W}^{ex} is equal to the dissipative Jarzynski work (in the β^{-1} units) $\beta(W - \Delta F)$ with W given by Eq.(7.20).

Example 13. The case of complete reversal. Recall that for the complete reversal rule of Sect. 6.6 based on the choice of densities $e^{-\varphi_t}$ evolving dynamically, \mathcal{J}_t is the total time derivative, see Eq.(7.14). The use in the definition (8.2) of the functions from the same family annihilates the functional \mathcal{W} :

$$\mathcal{W} \equiv 0. \quad (8.20)$$

9. Speck-Seifert Equality

Let us consider the two functionals \mathcal{W}^{tot} and \mathcal{W}^{ex} of the process \mathbf{x}_t introduced in Examples 11 and 12. We shall take them with the same functions φ_t satisfying $L_t^\dagger e^{-\varphi_t} = 0$. The two Jarzynski equalities $\langle e^{-\mathcal{W}^{tot}} \rangle = 1 = \langle e^{-\mathcal{W}^{ex}} \rangle$ hold simultaneously. In [78] a third equality of the same type, this time involving the quantity

$$\mathcal{W}^{hk} = \mathcal{W}^{tot} - \mathcal{W}^{ex} = \int_0^T [\nabla \varphi_t(\mathbf{x}_t) + 2 \hat{u}_t(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t)] \dot{\mathbf{x}}_t dt$$

was established in the context of the Langevin equation where $\mathcal{W}^{hk} = \beta Q^{hk} = \beta Q^{tot} - \beta Q^{ex}$ is the housekeeping heat (in the β^{-1} units). We shall prove here a generalization of the result of [78]. To this end, let us consider, besides the original process \mathbf{x}_t satisfying the SDE (2.1), the Markov process \mathbf{x}_t'' satisfying the same equation but with the drift \hat{u}_t replaced by

$$\hat{u}_t'' = -\hat{u}_t - d_t \nabla \varphi_t. \quad (9.1)$$

We shall denote by $\langle \cdot \rangle''$ the expectation defined by Eq. (8.4) but referring to the process \mathbf{x}_t'' . Note in passing the relations $L_t''^\dagger e^{-\varphi_t} = 0$, where the operators L_t'' are given by Eq. (3.3) with \hat{u}_t'' replacing \hat{u}_t . In particular, in the stationary case, the processes \mathbf{x}_t and \mathbf{x}_t'' have the same invariant measure.

Proposition 3.

$$\langle \mathcal{F} e^{-\mathcal{W}^{hk}} \rangle = \langle \mathcal{F} \rangle''. \quad (9.2)$$

Proof. The above identity may be proven directly with the use of the Cameron-Martin-Girsanov formula, see Appendix D, by comparing the measures of the processes \mathbf{x}_t and \mathbf{x}_t'' corresponding to SDEs differing by a drift term. Here we shall give another proof based on applying twice the relation (8.6). First, we use this relation with the functional \mathcal{F} replaced by $\mathcal{F} e^{-\mathcal{W}^{tot} + 2\mathcal{W}^{ex}}$ for the current-reversal time inversion with the trivial involution $x^* \equiv x$ and the vector-field rule for v_t . This results in the equality

$$\langle \mathcal{F} e^{-\mathcal{W}^{hk}} \rangle = \langle \tilde{\mathcal{F}} e^{-\tilde{\mathcal{W}}^{tot} + 2\tilde{\mathcal{W}}^{ex}} \rangle, \quad (9.3)$$

where the expectation $\langle \cdot \rangle$ pertains to the backward dynamics with

$$\hat{u}_t^i = -\hat{u}_{t^*}^i - d_{t^*}^{ij} \partial_j \varphi_{t^*}, \quad v_t^i = v_{t^*}^i,$$

see Eqs. (6.11). Now, we observe that the same backward process may be obtained by the reversed-protocol time inversion, again for $x^* \equiv x$, from the process \mathbf{x}_t'' introduced above. The identity (8.6) applied for the processes \mathbf{x}_t'' and \mathbf{x}_t' reads:

$$\langle \mathcal{F}'' e^{-\mathcal{W}''} \rangle' = \langle \tilde{\mathcal{F}}'' \rangle, \quad (9.4)$$

where

$$\mathcal{W}'' = \Delta\varphi + 2 \int_0^T \hat{u}_t''(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t) \dot{\mathbf{x}}_t dt$$

is the functional \mathcal{W} referring to the dynamics with $\hat{u}_t'' = \hat{u}_{t,+}''$ given by Eq. (9.1). The application of Eq. (9.4) to $\mathcal{F}'' = \mathcal{F} e^{-\mathcal{W}^{tot} + 2\mathcal{W}^{ex}}$ reduces the right hand side of Eq. (9.3) to the expectation $\langle \mathcal{F} e^{-(\mathcal{W}^{tot} - 2\mathcal{W}^{ex} + \mathcal{W}'')} \rangle'$. The equality (9.2) follows by checking that

$$\begin{aligned} \mathcal{W}^{tot} - 2\mathcal{W}^{ex} + \mathcal{W}'' &= \Delta\varphi + 2 \int_0^T \hat{u}_t(\mathbf{x}_t) \cdot d_t^{-1}(\mathbf{x}_t) \dot{\mathbf{x}}_t dt - 2 \int_0^T (\partial_t \varphi_t)(\mathbf{x}_t) dt \\ &\quad + \Delta\varphi + 2 \int_0^T (-\hat{u}_t(\mathbf{x}_t) - d_t(\mathbf{x}_t) \nabla \varphi_t(\mathbf{x}_t)) \cdot d_t^{-1}(\mathbf{x}_t) \dot{\mathbf{x}}_t dt \\ &= 2\Delta\varphi - 2 \int_0^T [\partial_t \varphi_t(\mathbf{x}_t) + \nabla \varphi_t(\mathbf{x}_t) \cdot \mathbf{x}_t] dt = 0. \end{aligned}$$

□

Setting $\mathcal{F} \equiv 1$ in the identity (9.2), we obtain the result that was established by a different argument in [78] in the context of the Langevin equation:

Corollary 3. (Speck-Seifert equality).

$$\left\langle e^{-\mathcal{W}^{hk}} \right\rangle = 1. \quad (9.5)$$

10. Entropy Production

An immediate consequence of the Jarzynski equality (8.7) and of the Jensen inequality (i.e. of convexity of the exponential function) is

Corollary 4. (2nd law of thermodynamics for diffusion processes).

$$\langle \mathcal{W} \rangle \geq 0. \quad (10.1)$$

To explain the relation of the latter inequality to the 2nd law of thermodynamics, let us first remark that the quantity on the left hand side has the interpretation of a relative entropy. Recall, that for two probability measures $\mu(d\mathbf{x})$ and $\nu(d\mathbf{x}) = e^{-w(\mathbf{x})} \mu(d\mathbf{x})$, the relative entropy of ν with respect to μ is defined by the formula

$$S(\mu|\nu) = \int w(\mathbf{x}) \mu(d\mathbf{x})$$

and is always non-negative. Now, the identity (8.6) may be read as the relation

$$\tilde{M}'(d\mathbf{x}) = e^{-\mathcal{W}} M(d\mathbf{x})$$

between the measures $M(d\mathbf{x})$ and $\tilde{M}'(d\mathbf{x}) \equiv M'(d\tilde{\mathbf{x}})$. In other words, $e^{-\mathcal{W}}$ is the relative (Radon-Nikodym) density of the trajectory measure \tilde{M}' with respect to the measure M . It follows that

$$\langle \mathcal{W} \rangle = S(M|\tilde{M}')$$

so that the inequality (10.1) expresses the positivity of the relative entropy.

Up to now, the measures μ_0 and μ_T were unrelated. Let us consider the particular case when μ_T is obtained by the dynamical evolution (3.6) from μ_0 so that $\mu_T = \mu_0 P_{0,T}$. In this case, the relative entropy $S(M|\tilde{M}')$ may be interpreted as the overall **entropy production** in the forward process between times 0 and T , relative to the backward process, see [27, 65, 39]. Let for a measure $\nu(dx) = \rho(x)dx$, $S(\nu) = -\int \ln \rho(x) \nu(dx)$ denotes its entropy. Using the definition (8.2), we may rewrite

$$\langle \mathcal{W} \rangle = S(\mu_T) - S(\mu_0) + \Delta S_{env}, \quad (10.2)$$

where the difference $S(\mu_T) - S(\mu_0)$ is the change of entropy of the fixed-time distribution of the process during the time T and

$$\Delta S_{env} = \int_0^T \langle \mathcal{J}_t \rangle dt. \quad (10.3)$$

The latter quantity will be interpreted as the mean entropy production in the environment modeled by the stochastic noise, measured relative to the backward process. The inequality (10.1) states that the overall entropy production cannot be negative in mean. In this sense, it is a version of the 2nd law of thermodynamics for the diffusion processes under consideration. In the stationary case, where $\mu_T = \mu_0$, the overall mean entropy production reduces to the one in the environment ΔS_{env} .

The rate of change of the fixed-time entropy $S(\mu_t)$ for $\mu_t = \mu_0 P_{0,t}$ is easily calculated with the use of Eq. (3.7) to be

$$\frac{dS(\mu_t)}{dt} = \int [\hat{u}_t \cdot \nabla \varphi_t + \frac{1}{2} (\nabla \varphi_t) \cdot d_t (\nabla \varphi_t)](x) \mu_t(dx) \quad (10.4)$$

for $\mu_t(dx) = e^{-\varphi_t(x)} dx$. Rewriting the expression (7.6) for \mathcal{J}_t in terms of the Itô convention, it is also easy to show that

$$\langle \mathcal{J}_t \rangle = \int [2 \hat{u}_{t,+} \cdot d_t^{-1} \hat{u}_{t,+} + (\nabla \cdot \hat{u}_{t,+}) - (\nabla \cdot u_{t,-})](x) \mu_t(dx). \quad (10.5)$$

The average (10.5) represents the instantaneous mean rate of the entropy production in the environment. Combining the last two expressions, we obtain the relation

$$\frac{dS(\mu_t)}{dt} + \langle \mathcal{J}_t \rangle = 2 \int [(\hat{u}_{t,+} + \frac{1}{2} d_t (\nabla \varphi_t)) \cdot d_t^{-1} (\hat{u}_{t,+} + \frac{1}{2} d_t (\nabla \varphi_t))](x) \mu_t(x) \quad (10.6)$$

which is explicitly positive. This provides still another proof of the positivity of the expectation $\langle \mathcal{W} \rangle$ which is the time integral of the latter expression if the measure μ_T is obtained by evolving dynamically μ_0 . See Eq. (13) in [66] for the special case of the latter relation. If $\mu_T \neq \mu_0 P_{0,T}$ then one has to distinguish between those two measures and the relation (10.2) is modified to

$$\langle \mathcal{W} \rangle = S(\mu_0 P_{0,T}) - S(\mu_0) + \Delta S_{env} + S(\mu_0 P_{0,T} | \mu_T),$$

i.e. the right hand side is increased by the relative entropy of the measure μ_T with respect to the measure obtained from μ_0 by the dynamical evolution. Consequently, the average $\langle \mathcal{W} \rangle$ is minimal when $\mu_T = \mu_0 P_{0,T}$.

Note that ΔS_{env} as defined by Eq. (10.3) depends on the time inversion employed (more precisely, on the splitting of μ_t), and the quantities obtained by employing different time inversions are, in general, different. They may have different physical relevance. We may talk about the total mean entropy production in the environment

$$\Delta S_{env}^{tot} = \int_0^T \langle \mathcal{J}_t^{tot} \rangle dt = \int_0^T dt \int [2 \hat{u}_t \cdot d_t^{-1} \hat{u}_t + (\nabla \cdot \hat{u}_t)](x) \mu_t(dx),$$

if the reversed protocol of Sect. 6.4 and Example 11 is used or about the excess mean entropy production

$$\Delta S_{env}^{ex} = \int_0^T dt \int [\nabla \cdot \hat{u}_t - 2 \hat{u}_t \cdot (\nabla \varphi_t) - \frac{1}{2} (\nabla \varphi_t) \cdot d_t (\nabla \varphi_t)](x) \mu_t(dx)$$

in the environment for the current reversal of Sect. 6.5 and Example 12 (in the latter formula, $e^{-\varphi_t}$ satisfies $L_t^\dagger e^{-\varphi_t} = 0$ and is, in general different from the density of $\mu_t = \mu_0 P_{0,t}$). The Speck-Seifert equality (9.5) combined with the Jensen inequality imply that ΔS_{env}^{ex} does not exceed ΔS_{env}^{tot} which may be also seen directly since

$$\begin{aligned} \Delta S_{env}^{tot} - \Delta S_{env}^{ex} &= \langle \mathcal{W}^{hk} \rangle \\ &= 2 \int_0^T dt \int \left[(\hat{u}_t + \frac{1}{2} d_t \cdot (\nabla \varphi_t)) \cdot d_t^{-1} (\hat{u}_t + \frac{1}{2} d_t \cdot (\nabla \varphi_t)) \right](x) \mu_t(dx) \geq 0. \end{aligned}$$

As an illustration, consider the stationary Langevin equation with the vanishing additional force where $\Delta S_{env}^{ex} = 0$ although ΔS_{env}^{tot} may be non-zero if $\Pi \neq 0$. In particular, in the linear case studied in Example 8,

$$\Delta S_{env}^{tot} = \int_0^T \langle \mathcal{J}_t^{tot} \rangle dt = \int_0^T \langle \beta \mathbf{x}_t \cdot M^T \Gamma^{-1} M \mathbf{x}_t + \text{tr } M \rangle dt = -T \text{tr } \Pi \Gamma^{-1} M$$

by Eq. (10.5).

For the general diffusion process and the drift splitting corresponding to the modified natural time inversion of Sect. 6.2, i.e. for $\hat{u}_{t,+} \equiv 0$,

$$\Delta \widehat{S}_{env}^{nat} = \int_0^T \langle \widehat{\mathcal{J}}_t^{nat} \rangle dt = - \int_0^T dt \int (\nabla \cdot \hat{u}_t)(x) \mu_t(dx), \quad (10.7)$$

see Eq. (8.10). The difference

$$\Delta S_{env}^{tot} - \Delta S_{env}^{\widehat{nat}} = 4 \int_0^T \mathcal{T}(\mu_t) dt, \quad (10.8)$$

where the functional

$$\mathcal{T}(\mu_t) = \frac{1}{2} \int [\hat{u}_t \cdot d_t^{-1} \hat{u}_t + (\nabla \cdot \hat{u}_t)](x) \mu_t(dx) \quad (10.9)$$

was called the **traffic** in [66].

For the Langevin equation with the splitting (6.7) corresponding to the canonical time inversion, the entropy production in the environment is proportional to the mean heat transferred to the environment as given by Eq. (7.16):

$$\Delta S_{env}^{Lan} = \beta \langle Q \rangle = \int_0^T dt \int [\beta (\nabla H_t)(x) \cdot \Gamma(\nabla H_t)(x) - \Gamma^{ij} \partial_i \partial_j H(x) - (\nabla \cdot G_t)(x)] \mu_t(dx).$$

In the deterministic case when \mathcal{J}_t is given by Eq. (8.11), the mean rate of entropy production in the environment is

$$\langle \mathcal{J}_t^{det} \rangle = - \int (\nabla \cdot u_t)(x) \mu_t(dx)$$

for $\mu_t = \mu_0 P_{0,t}$ obtained by the dynamical evolution from μ_0 with $P_{0,t}(\mathbf{x}_0, dy) = \delta(y - \mathbf{x}_t) dy$. For uniformly hyperbolic dynamical systems without explicit time dependence, the measures μ_t tend for large t to the invariant SRB measure μ_∞ and the mean rate of entropy production in the environment converges to the expectation of the phase-space contraction rate $-\nabla \cdot u$ with respect to μ_∞ [74]. A discussion of the relation between of the phase-space contraction and the production of thermodynamic entropy in deterministic dynamics employing models of finite-dimensional thermostats may be found in [33].

Finally, let us remark that if the complete reversal of Sect. 6.6 is employed to define the backward process then the overall entropy production vanishes because $\mathcal{W} \equiv 0$ in this case, see Eq. (8.20). With our flexibility of the choice of backward processes, there are always ones with respect to which there is no overall entropy production!

11. Linear Response for the Langevin Dynamics

11.1. Green-Kubo formula and Onsager reciprocity. As noted in [23, 32, 59], fluctuation relations may be viewed as extensions to the non-perturbative regime of the Green-Kubo and Onsager relations for the nonequilibrium transport coefficients valid within the linear response description of the vicinity of the equilibrium. Here, for the sake of completeness, we shall show how such relations follow formally from the Jarzynski equality (8.7) for the Langevin dynamics. To this end, we shall consider the latter with a time independent Hamiltonian $H_t \equiv H$ and the additional time-dependent force

$$G_t(x) = g_{ta} G^a(x),$$

where the couplings g_{ta} , $a = 1, 2$, are arbitrary (regular) functions of time (and the summation over the index a is understood). In the case at hand, we infer from Eq. (8.8) that

$$\mathcal{W} = \int_0^T g_{ta} J^a(\mathbf{x}_t) dt \quad \text{for} \quad J^a = \beta(\nabla H) \cdot G^a - \nabla \cdot G^a.$$

In particular, for the Langevin-Kramers equation (2.7),

$$J^a = \beta f_i^a(q) \dot{q}^i$$

is the power injected by the external force f^a (in the β^{-1} units). The quantities J^a are often called **fluxes** associated to the forces G^a .

Let us denote by $\langle \mathcal{F} \rangle$ the expectation defined by Eq. (8.4) with μ_0 standing for the Gibbs measure $Z^{-1}e^{-\beta H}dx$ and by $\langle \mathcal{F} \rangle_0$ the same expectation taken for $g_{ta} \equiv 0$, i.e. in the equilibrium system. Expanding Eq. (8.7) up to the second order in g_{ta} and abbreviating $J^a(\mathbf{x}_t) \equiv J_t^a$, we obtain the identity

$$-\int_0^T g_{ta} \langle J_t^a \rangle_0 dt - \int_0^T \int_0^T g_{ta} g_{tb} \langle J_t^a \mathcal{R}_{t'}^b \rangle_0 dt dt' + \frac{1}{2} \int_0^T \int_0^T g_{ta} g_{tb} \langle J_t^a J_{t'}^b \rangle_0 dt dt' = 0, \quad (11.1)$$

where the insertion of the response field \mathcal{R}_t^a is defined by the relation

$$\langle \mathcal{F} \mathcal{R}_t^a \rangle_0 = \left. \frac{\delta}{\delta g_{ta}} \right|_{g=0} \langle \mathcal{F} \rangle.$$

Note that $\langle J_t^a \mathcal{R}_{t'}^b \rangle_0 = 0$ for $t' > t$ because of the causal nature of the stochastic evolution. The vanishing of the term linear in g_{ta} in Eq. (11.1) implies that the equilibrium expectation of the fluxes J^a vanishes

$$\langle J_t^a \rangle_0 = Z^{-1} \int J^a(x) e^{-\beta H(x)} dx = 0,$$

which is easy to check directly. Stripping the quadratic term in Eq. (11.1) of arbitrary functions g_{ta} , we infer that

$$\langle J_t^a \mathcal{R}_{t'}^b \rangle_0 = \theta(t - t') \langle J_t^a J_{t'}^b \rangle_0.$$

The integration of the latter equation over $t' \geq 0$ results in the relation

$$\left. \frac{\partial}{\partial g_b} \right|_{g=0} \langle J_t^a \rangle = \int_0^t \langle J_t^a J_{t'}^b \rangle_0 dt', \quad (11.2)$$

where on the left hand side we consider the derivative with respect to the coupling g_b constant in time. In the limit $t \rightarrow \infty$, we may expect the convergence of the expectation $\langle J_t^a \rangle$ in the presence of the time-independent force $g_a G^a$ (and of its derivatives over g_b) to the nonequilibrium stationary expectation $\langle J_t^a \rangle_{st}$ (and its derivatives). Let us also assume that the temporal decay of the stationary equilibrium correlation function of the fluxes is sufficiently fast, e.g. exponential. These may be often established for the dynamics governed by the Langevin equation by studying the properties of its generator. With these assumptions, Eq. (11.2) implies

Proposition 4. (Green-Kubo formula).

$$\left. \frac{\partial}{\partial g_b} \right|_{g=0} \langle J_t^a \rangle_{st} = \int_{-\infty}^t \langle J_t^a J_{t'}^b \rangle_0 dt'.$$

The stationary equilibrium correlation function $\langle J_t^a J_{t'}^b \rangle_0$ depends only on the difference $t - t'$ of times. Besides, if the system is time-reversible, then $\langle J_t^a J_{t'}^b \rangle_0 = \langle J_t^b J_{t'}^a \rangle_0$ and the Green-Kubo formula may be rewritten in the form

$$\left. \frac{\partial}{\partial g_b} \right|_{g=0} \langle J_t^a \rangle_{st} = \frac{1}{2} \int \langle J_t^a J_{t'}^b \rangle_0 dt' = \frac{1}{2} \int \langle J_t^b J_{t'}^a \rangle_0 dt'$$

which implies

Corollary 5. (Onsager reciprocity).

$$\left. \frac{\partial}{\partial g_b} \right|_{g=0} \langle J_t^a \rangle_{st} = \left. \frac{\partial}{\partial g_a} \right|_{g=0} \langle J_t^b \rangle_{st}.$$

11.2. Fluctuation-dissipation theorem. Let us consider again the Jarzynski equality for the Langevin dynamics, this time in the absence of the additional force G_t but with a time dependent Hamiltonian

$$H_t(x) = H(x) - h_{ta} O^a(x), \quad (11.3)$$

where h_{ta} , $a = 1, 2$, vanish at $t = 0$ and $O^a(x)$ are functions of x (“observables”). In this case, Eq. (8.8) reduces to the relation

$$\mathcal{W} = -\beta \int_0^T \dot{h}_{ta} O^a(\mathbf{x}_t) - \beta \Delta F,$$

where

$$\beta \Delta F = -\ln \int e^{-\beta(H(x) - h_{Ta} O^a(x))} dx + \ln \int e^{-\beta H(x)} dx.$$

Expanding the left hand side of the Jarzynski equality (8.7) up to the second order in h_{ta} and abbreviating $O^a(\mathbf{x}_t) \equiv O_t^a$, we infer that

$$\beta \int_0^T \dot{h}_{ta} \langle O_t^a \rangle_0 dt - \beta h_{Ta} \langle O_0^a \rangle_0 = 0 \quad (11.4)$$

and that

$$\begin{aligned} \frac{1}{2} \beta^2 \int_0^T \int_0^T \dot{h}_{ta} \dot{h}_{t'b} \langle O_t^a O_{t'}^b \rangle_0 dt dt' + \beta \int_0^T \int_0^T \dot{h}_{ta} h_{t'b} \langle O_t^a R_{t'}^b \rangle_0 dt dt' \\ - \frac{1}{2} \beta^2 h_{Ta} h_{Tb} \langle O_0^a O_0^b \rangle_0 = 0, \end{aligned} \quad (11.5)$$

where the insertion of the response field R_t^a is defined similarly as that of \mathcal{R}_t^a before by

$$\langle \mathcal{F} R_t^a \rangle_0 = \frac{\delta}{\delta h_{ta}} \Big|_{h=0} \langle \mathcal{F} \rangle.$$

Again, similarly as before, $\langle O_t^a R_{t'}^b \rangle_0 = 0$ for $t' > t$ because of causality.

The first order equality (11.4) is equivalent to the time-independence of the equilibrium expectation of O_t^a . As for the second order relation (11.5), upon expressing h_{ta} as the integral of \dot{h}_{ta} , it is turned into the equality

$$\beta \int_0^T \int_0^T \dot{h}_{ta} \dot{h}_{t'b} \langle (O_t^a O_t^b - O_t^a O_{t'}^b) \rangle_0 dt dt' = 2 \int_0^T \int_0^T \int_0^{t'} \dot{h}_{ta} \dot{h}_{t''b} \langle O_t^a R_{t''}^b \rangle_0 dt dt' dt''.$$

After the change of the order of integration over t' and t'' followed by the interchange of those symbols, the right hand side becomes

$$2 \int_0^T \int_0^T \int_{t'}^t \dot{h}_{ta} \dot{h}_{t'b} \langle O_t^a R_{t''}^b \rangle_0 dt dt' dt'' = 2 \int_0^T \int_0^T \int_{t'}^t \dot{h}_{ta} \dot{h}_{t'b} \theta(t - t') \langle O_t^a R_{t''}^b \rangle_0 dt dt' dt''$$

with the use of causality. Stripping the resulting identity of the integrals against arbitrary functions \dot{h}_{ta} , we obtain the identity

$$\beta \langle O_t^a O_t^b \rangle_0 - \beta \langle O_t^a O_{t'}^b \rangle_0 = \theta(t - t') \int_{t'}^t \langle O_t^a R_{t''}^b \rangle_0 dt'' + \theta(t' - t) \int_t^{t'} \langle O_{t'}^a R_{t''}^b \rangle_0 dt''$$

which is the integrated version of the differential relation between the dynamical 2-point correlation function and the response function:

Proposition 5. (Fluctuation-dissipation theorem). *For $t > t'$,*

$$-\partial_t \langle O_t^a O_{t'}^b \rangle_0 = \beta^{-1} \langle O_t^a R_{t'}^b \rangle_0. \quad (11.6)$$

Note the explicit factor β in this identity. Relations between the dynamical correlation functions and the response functions were used in recent years to extend the concept of temperature to nonequilibrium systems [20, 14].

12. One-Dimensional Langevin Equation with Flux Solution

Let us consider, as an illustration, the one-dimensional Langevin equation of the form

$$\dot{x} = -\partial_x H_t(x) + \zeta_t \quad (12.1)$$

with $\langle \zeta_t \zeta_{t'} \rangle = 2\beta^{-1} \delta(t - t')$ (any force is a gradient in one dimension). As before, \mathbf{x}_t will represent the Markov process solving the SDE (12.1). First, let us consider the time-independent case with a polynomial Hamiltonian $H(x) = ax^k + \dots$ with $a \neq 0$ and the dots representing lower order terms.

- If $k = 0$ then, up to a linear change of variables, \mathbf{x}_t is a Brownian motion and does not have an invariant probability measure.
- If $k = 1$ then $\mathbf{x}_t + at$ is, up to a linear change of variables, a Brownian motion and \mathbf{x}_t still does not have an invariant probability measure.

- If $k \geq 2$ and is even then for $a > 0$ the Gibbs measure $\mu_0(dx) = Z^{-1}e^{-\beta H(x)}dx$ provides the unique invariant probability measure of the process \mathbf{x}_t . It satisfies the detailed balance condition $j(x) = 0$, where $j(x)$ is the probability current defined by Eq. (3.8). If $a < 0$, however, then the Gibbs density $e^{-\beta H(x)}$ is not normalizable⁴. In this case, the process \mathbf{x}_t escapes to $\pm\infty$ in finite time with probability one and it has no invariant probability measure.
- If $k \geq 3$ and is odd then the Gibbs density $e^{-\beta H(x)}$ is not normalizable. The process \mathbf{x}_t escapes in finite time to $-\infty$ if $a > 0$ and to $+\infty$ if $a < 0$, but it has a realization with the trajectories that reappear immediately from $\pm\infty$. Such a resuscitating process has a unique invariant probability measure

$$\mu_0(dx) = \pm N^{-1} \left(e^{-\beta H(x)} \int_{\mp\infty}^x e^{\beta H(y)} dy \right) dx \equiv e^{-\varphi_0(x)} dx \quad (12.2)$$

with the density $e^{-\varphi_0(x)} = \mathcal{O}(x^{-k+1})$ when $x \rightarrow \pm\infty$ and N the (positive) normalization constant. The measure μ_0 corresponds to a constant probability current $j(x) = \mp(\beta N)^{-1}$ and the model provides the simplest example on a nonequilibrium steady state with a constant flux.

Let us look closer at the last case. Adding the time-dependence and taking φ_t as in Eq. (12.2) but with H_t replacing H , we obtain the Hatano-Sasa version of the Jarzynski equality (8.7) with $\mathcal{W} = \mathcal{W}^{ex}$ given by Eq. (8.19). Suppose, in particular, that the time dependence of H_t has the form (11.3) with functions O^a having compact support. Let us introduce also the deformed observables

$$\widehat{O}^a(x) = \frac{\int_{\mp\infty}^x O^a(y) e^{\beta H(y)} dy}{\int_{\mp\infty}^x e^{\beta H(y)} dy}.$$

Expanding the Jarzynski identity (8.7) to the second order in h_{at} as in Sect. 11.2, one obtains:

Proposition 6. (Deformed fluctuation-dissipation relation). *For $t > t'$,*

$$-\partial_t \langle A_t^a O_{t'}^b \rangle_0 = \beta^{-1} \langle A_t^a R_{t'}^b \rangle_0 \\ \mp (\beta N)^{-1} \int (\partial_x O^b)(x) dx P_{t-t'}(x, dy) A^a(y), \quad (12.3)$$

where $P_t(x, dy)$ is the transition probability in the stationary process and $A^a = O^a - \widehat{O}^a$.

Remark 3. It is easy to show directly, that Eq. (12.3) still holds if A^a is replaced by O^a . Note that the term on the right hand side of (12.3) violating the standard fluctuation-dissipation theorem (11.6) contains the constant flux of the probability current $j(x)$ as a factor. Proof of Proposition 6 and of its version with A^a replaced by O^a will be given in [12].

⁴ This leads to the breaking of the quantum-mechanical supersymmetry underlying the Fokker-Planck formulation of the Langevin dynamics [85, 69, 80].

The Langevin equation (12.1) with the flux solution arises when one studies the tangent process for particles with inertia moving in the one-dimensional homogeneous Kraichnan ensemble of velocities $v_t(y)$ with the covariance

$$\langle v_t(y) v_s(y') \rangle = \delta(t-s) D(y-y'),$$

see Example 2. The position y and the velocity w of such particles satisfy the SDE [3]

$$\dot{y} = w, \quad \dot{w} = \frac{1}{\tau}(-w + v_t(y)),$$

where τ is the so called Stokes time measuring the time-delay of particles with inertia as compared to the Lagrangian particles that follow the flow. The separation between two infinitesimally close trajectories of particles satisfies the equations [84]

$$\frac{d}{dt} \delta y = \delta w, \quad \frac{d}{dt} \delta w = \frac{1}{\tau}(-\delta w + (\partial_y v_t)(y) \delta y) \quad (12.4)$$

and, similarly as in Example 5, we may replace $\frac{1}{\tau} \partial_y v_t(y)$ on the right hand side by a white noise $\zeta(t)$ with the covariance

$$\langle \zeta_t \zeta_s \rangle = -\delta(t-s) \tau^{-2} D''(0),$$

where the primes denote the spatial derivatives. The ratio $x = \frac{\delta w}{\delta y}$ satisfies then the SDE

$$\dot{x} = -x^2 - \frac{1}{\tau} x + \zeta_t \quad (12.5)$$

which has the form (12.1) with $H(x) = \frac{1}{3}x^3 + \frac{1}{2\tau}x^2$, a third order polynomial. The solution with the trajectories appearing at $+\infty$ after disappearing at $-\infty$ corresponds to the solution for $(\delta y, \delta w)$ with δy passing through zero with positive speed. The top Langevin exponent for the random dynamical system (12.4) is obtained as the mean value of x (which is the temporal logarithmic derivative of $|\delta y|$) in the invariant probability measure (12.2) with constant flux [84].

A very similar SDE arose earlier [41] in the one-dimensional Anderson localization in white-noise potential $V(y)$, where one studies the stationary Schrödinger equation

$$-\psi''(y) + V(y) \psi(y) = E \psi(y).$$

By setting $x = \psi'/\psi$, one obtains then the evolution SDE

$$x' = -x^2 - E + V(y) \quad (12.6)$$

that has an invariant probability measure with constant flux, as already noticed in [41]. The expectation value of x in that measure may be expressed by the Airy functions [61]. It gives the (top) Lyapunov exponent which is always positive, reflecting the permanent localization in one dimension. The SDE (12.5) may be obtained from (12.6) but taking in the latter $E = -\frac{1}{4\tau^2}$ and by the substitutions $x - \frac{t}{2\tau} \mapsto x$, $V \mapsto \zeta$ and $y \mapsto t$. This shifts the Lyapunov exponent down by $-\frac{1}{2\tau}$ and the top exponent for the inertial particles may have both signs [84].

13. Detailed Fluctuation Relation

For a general pair of forward and backward diffusion processes (2.1) and (5.4), it is still possible to obtain identities resembling the generalized detailed balance relation (7.15) at the price of adding constraints on the process trajectories. Let us introduce a functional \mathcal{W}' of the backward process by mimicking the definition (8.2) of \mathcal{W} for the forward process:

$$\mathcal{W}' = \Delta\varphi' + \int_0^T \mathcal{J}'_t dt$$

with

$$\mathcal{J}'_t = 2\hat{u}'_{t,+}(\mathbf{x}'_t) \cdot d'^{-1}(\mathbf{x}'_t) \dot{\mathbf{x}}'_t - 2\hat{u}'_{t,+}(\mathbf{x}'_t) \cdot d'^{-1}(\mathbf{x}'_t) u'_{t,-}(\mathbf{x}'_t) - (\nabla \cdot u'_{t,-})(\mathbf{x}'_t),$$

see Eq. (7.6). Since the time inversion is involutive, the mirror version of the identity (8.3),

$$\mu'_0(dx') \mathbf{E}_{x',y'}^{0,T} \mathcal{F}'(\mathbf{x}') e^{-\mathcal{W}'(\mathbf{x}')} dy' = \mu_0(dy^*) \mathbf{E}_{y'^*,x'^*}^{0,T} \tilde{\mathcal{F}}'(\mathbf{x}) dx'^* dx'^*, \quad (13.1)$$

must also hold. Taking $x' = y^*$, $y' = x^*$ and $\mathcal{F}' = \tilde{\mathcal{F}} e^{-\tilde{\mathcal{W}}}$, we infer that the compatibility of identities (8.3) and (13.1) imposes the equality

$$\mathcal{W}' = -\tilde{\mathcal{W}}, \quad (13.2)$$

which may be also checked directly. We infer that, whatever the time inversion used in their definition, the entropy-production functionals \mathcal{W} for the forward and the backward processes are related by the natural time inversion. The replacement in Eq. (8.3) of the functional $\mathcal{F}(\mathbf{x})$ by the functional $\mathcal{F}(\mathbf{x}) \delta(\mathcal{W}(\mathbf{x}) - W)$ including the constraint fixing the value of \mathcal{W} , leads then to

Proposition 7. (Detailed fluctuation relation).

$$\begin{aligned} \mu_0(dx) \mathbf{E}_{x,y}^{0,T} \mathcal{F}(\mathbf{x}) \delta(\mathcal{W}(\mathbf{x}) - W) dy &= \mu'_0(dy^*) e^{\mathcal{W}} \\ &\times \mathbf{E}_{y'^*,x'^*}^{0,T} \tilde{\mathcal{F}}(\mathbf{x}') \delta(\mathcal{W}'(\mathbf{x}') + W) dx^*. \end{aligned} \quad (13.3)$$

The primes on the right hand side may be dropped in the time-reversible case if, additionally, $\varphi_0 = \varphi'_0$ and $\varphi_T = \varphi'_T$. \square

A relation of this type, named the “detailed fluctuation theorem”, was established in [51] in the setup of Hamiltonian dynamics. It is close in spirit to the earlier observation made for the long-time asymptotics of deterministic dynamical systems in [31]. We shall view Proposition 7 as a source of fluctuation relations that hold for the diffusion processes (2.1), including the Jarzynski equality (8.7) already discussed and various identities that appeared in the literature in different contexts, see [51, 18, 19, 57]. Taking, in particular, $\mathcal{F} \equiv 1$ in Eq. (13.3) and introducing the joint probability distributions of the end-point of the process and of the entropy production functional \mathcal{W} ,

$$\begin{aligned} \mathbf{E}_{x,y}^{0,T} \delta(\mathcal{W}(\mathbf{x}) - W) dy dW &= P_{0,T}(x, dy, dW), \\ \mathbf{E}_{x,y}^{0,T} \delta(\mathcal{W}'(\mathbf{x}') - W') &= P'_{0,T}(x, dy, dW'), \end{aligned}$$

we obtain

Corollary 6.

$$\mu_0(dx) P_{0,T}(x, dy, dW) = \mu_T(dy) e^W P'_{0,T}(y^*, dx^*, d(-W)). \quad (13.4)$$

This may be viewed as an extension to a general diffusive SDE (2.1) of the detailed balance relation (3.9), or of its generalization (7.15). In particular, when the backward process is obtained by the complete reversal of Sect. (6.6) with $\mathcal{W} \equiv 0$, the latter relation reduces to Eq. (7.15) with both sides multiplied by $\delta(W)dW$.

In the case when the measures μ_0 and μ'_0 are normalized, Proposition 7 gives rise, upon integration over x and y , to a detailed fluctuation relation between the forward and the backward processes with the initial points sampled with measures μ_0 and μ'_0 , respectively:

Corollary 7.

$$\left\langle \mathcal{F} \delta(\mathcal{W} - W) \right\rangle = e^W \left\langle \tilde{\mathcal{F}} \delta(\mathcal{W}' + W) \right\rangle.$$

Finally, taking $\mathcal{F} = 1$ in the latter identity and denoting

$$p_{0,T}(dW) = \left\langle \delta(\mathcal{W} - W) \right\rangle dW, \quad p'_{0,T}(dW') = \left\langle \delta(\mathcal{W}' - W') \right\rangle dW',$$

we obtain

Corollary 8. (Crooks relation) [18, 19].

$$p_{0,T}(dW) = e^W p'_{0,T}(d(-W)). \quad (13.5)$$

Note that $p_{0,T}(dW)$ is the distribution of the random variable \mathcal{W} if the time-zero values of the forward process \mathbf{x}_t are distributed with the measure μ_0 and, similarly, $p'_{0,T}(dW')$ is the distribution of the random variable \mathcal{W}' if \mathbf{x}'_0 is distributed with the measure μ'_0 . In particular, in the time-reversible case, $p'_{0,T}(dW) = p_{0,T}(dW)$ if $\varphi'_0 = \varphi_0$ and $\varphi'_T = \varphi_T$. Finally, note that integrating the Crooks relation (13.5) multiplied by e^{-W} over W , one recovers the Jarzynski equality (8.7).

14. Special Cases

14.1. Deterministic case. As already explained in Sect. 6.2 and 13, taking $\hat{u}_{t,+} = 0$ and $u_{t,-} = \hat{u}_t$ leads in the limit of the deterministic dynamics (2.3) to the expression (8.12) for \mathcal{W} . The time-reversed dynamics corresponds to the vector fields of Eqs. (6.2). It reduces in the deterministic case to the ODE (6.3). The functional \mathcal{W}' of the backward process, that could be also found from the relation (13.2), takes the form

$$\mathcal{W}' = \Delta\varphi' + \int_0^T [(\nabla \ln \sigma)(\mathbf{x}'_t) \cdot (\dot{\mathbf{x}}'_t - u'_{t,-}) - (\nabla \cdot u'_{t,-})(\mathbf{x}'_t)] dt.$$

In the deterministic limit, this simplifies to the expression

$$\mathcal{W}' = \Delta\varphi' - \int_0^T (\nabla \cdot u'_t)(\mathbf{x}'_t) dt$$

which is of the same form as Eq.(8.12) for \mathcal{W} . Proposition 7 and Corollaries 6,7 and 8 still hold in the deterministic limit. In particular, in the time-reversible deterministic case with $u' = u$ and $\varphi_T = \varphi_0 = \varphi'_0$, the fluctuation relation (13.5) reduces to

Corollary 9. (Evans-Searles transient fluctuation theorem) [25,26].

$$p_{0,T}(dW) = e^W p_{0,T}(d(-W)).$$

The latter relation may also be proven directly by a change of the integration variables $\mathbf{x}_0 \mapsto \mathbf{x}_t$ [26].

14.2. Reversed protocol case. For the reversed protocol time inversion of Sect. 6.4 and Example 11 that corresponds to the choice (6.8), the backward process is given by Eq. (6.9) and

$$\mathcal{W}' = \Delta\varphi' + 2 \int_0^T \hat{u}'_t(\mathbf{x}'_t) \cdot d'^{-1}_t(\mathbf{x}'_t) \dot{\mathbf{x}}'_t dt$$

and has the same form as \mathcal{W} , see Eq.(8.14). For such a time inversion with $x^* \equiv x$, employed already in the stationary context in [59], the fluctuation relation (13.5) for the choice of φ_t such that $L_t^\dagger e^{-\varphi_t} = 0$ was established in [10].

14.3. Current reversal case. For the time inversion (6.10) discussed in Sect. 6.5 and Example 12, the functional \mathcal{W}' of the backward process is given by the expression of the same form as Eq.(8.19):

$$\mathcal{W}' = \int_0^T (\partial_t \varphi'_t)(\mathbf{x}'_t) dt$$

for $\varphi'_t(x) = (\varphi_{t*} + \ln \sigma)(x^*)$. The fluctuation relation (13.5) for this type of time inversion (with $x^* \equiv x$) was proven in [10]. Integrated against e^{-W} , Eq.(13.5) reduces to the Hatano-Sasa case of the Jarzynski equality (8.7) that we discussed in Example 12.

14.4. Langevin dynamics case. Recall that for the Langevin dynamics (2.4), the backward process obtained by using a canonical time inversion defined by Eqs.(6.6) and (6.7) is also of the Langevin type with

$$u'_t = -\Gamma \nabla H'_t + \Pi \nabla H'_t + G'_t, \quad (14.1)$$

where $H'_t(x) = H_{t*}(rx)$, $G'_t(x) = -rG_{t*}(rx)$. The white noise $\zeta'_t = \pm r\zeta_{t*}$ has the same distribution as ζ_t . Consequently, for $\varphi'_t = \beta(H'_t - F'_t)$, the functional \mathcal{W}' is given by the primed version of Eq. (8.8) and is equal to the dissipative work (in the β^{-1} units).

If, instead of the canonical time inversion, we use the reversed protocol with $x^* \equiv x$, then the backward process is again the Langevin dynamics with u'_t given by Eq.(14.1), except that this time $H'_t(x) = H_{t*}(x)$ and $G'_t(x) = G_{t*}(x)$. The white noise $\zeta'_t = \zeta_{t*}$

has again the same distribution as ζ_t . The functional \mathcal{W}' is given in that case by the primed version of Eq. (8.15). The two time inversions lead to the equivalent backward processes for the Langevin-Kramers equation but, as already mentioned, \mathcal{W}^{tot} is not well defined in the case of the reversed protocol.

Finally, if we apply the current-reversal time inversion (6.10) with $x^* \equiv x$ to the Langevin dynamics (2.4) with $G_t \equiv 0$ by setting $\varphi_t = \beta(H_t - F_t) = \varphi'_{t*} = \beta(H'_{t*} - F'_{t*})$ for $H'_t(x) = H_{t*}(x)$, the drift of the backward dynamics becomes

$$u'_t = -\Gamma \nabla H'_t - \Pi \nabla H'_t$$

and has the changed sign of the antisymmetric matrix Π with respect to the forward process. The white noise $\zeta'_t = \pm \zeta_{t*}$. Here both \mathcal{W} and \mathcal{W}' have the form of the dissipative work.

15. Transient Versus Stationary Fluctuation Relations

The fluctuation relations considered up to now dealt with the quantities related to finite-time evolution in a random process that, in general, was not stationary. Such simple relations, whose prototypes were the Evans-Searles fluctuation relation [25] or the Jarzynski equality [48] are called **transient** fluctuation relations. On the other hand, as was recalled in Introduction, Gallavotti and Cohen have established in [35] a fluctuation relation for quantities pertaining to the long-time evolution in stationary deterministic dynamical systems of chaotic type and similar relations were subsequently obtained for the Langevin dynamics and Markov processes in [57] and [59]. Such fluctuation relations, that are commonly termed **stationary**, are usually more difficult to establish than the transient ones and require some non-trivial work that involves the existence and the properties of the stationary regime of the dynamics. Such properties are in general harder to establish in the non-random case than in the random one. Also, in the random case, the invariant measure of the process, if it exists, is usually smooth. It could be used as the measure $\mu_0(dx) = e^{-\varphi_0(x)}dx = \mu_T(dx) = \mu'_0(dx^*)$ in the definition (8.2), leading to the exact detailed fluctuation relation (13.3) pertaining to the stationary evolution. On the other hand, in the dissipative deterministic systems, the invariant (SRB) measures are not smooth, so that they may not be used this way and the exact stationary fluctuation relations may be obtained only in the asymptotic long-time regime. Let us discuss briefly a formal relation between such asymptotic fluctuation relations and the transient ones, sweeping under the rug the hard points.

We shall consider the stationary case of the SDE (2.1), with $u_t \equiv u$ and $D_t(x, y) \equiv D(x, y)$. Under precise conditions, the Markov process \mathbf{x}_t that has decaying dynamical correlations and attains at long times the steady state independent of the initial (or/and final) position [42,55]. In such a situation, the distribution of the functional \mathcal{W} is expected (and may often be proven with some work) to take for long time T and for $\mathcal{W}/T = \mathcal{O}(1)$ the large deviation form

$$P_{0,T}(x, dy, dW) \propto e^{-T\zeta(\mathcal{W}/T)} dy dW \quad (15.1)$$

independent of x and y . The function ζ is called the large deviations rate function. It has vanishing minimum. More exactly, the relation (15.1) means that

$$\begin{aligned}
 -\sup_{w \in \mathcal{I}} \zeta(w) &\leq \varliminf_{T \rightarrow \infty} \frac{1}{T} \ln \int_{T\mathcal{I}} P_{0,T}(x, y | \mathcal{W}) d\mathcal{W} \\
 &\leq \varliminf_{T \rightarrow \infty} \frac{1}{T} \ln \int_{T\mathcal{I}} P_{0,T}(x, y | \mathcal{W}) d\mathcal{W} \leq -\inf_{w \in \mathcal{I}} \zeta(w)
 \end{aligned}$$

for any interval \mathcal{I} in the real line. In particular, in the limit $T \rightarrow \infty$, the distribution of \mathcal{W}/T concentrates at the non-random value w_0 , where the rate function ζ attains its minimum. With similar assumptions about the inverse process, we shall denote by ζ' the large deviation rate function of the functional \mathcal{W}' . The detailed fluctuation relation (13.4) implies then immediately, if the boundary term $\varphi'_0(y^*)/T = (\varphi_T(y) + \ln \sigma(y))/T$ converges to zero when $T \rightarrow \infty$, a relation between the rate functions ζ and ζ' :

Corollary 10. (Stationary fluctuation relation).

$$\zeta(w) = \zeta'(-w) - w. \quad (15.2)$$

Equation (15.2) connects the statistics of large deviations of \mathcal{W} for the forward and for the backward stationary stochastic processes. Note that the equality $\zeta' \geq 0$ implies that the asymptotic value w_0 of \mathcal{W}/T is non-negative. This conclusion may be also drawn from the 2nd law (10.1). In the special case of a stationary time-reversible dynamics, the inverse process coincides with the direct one so that $\zeta' = \zeta$. Equation (15.2) compares then the large deviations of \mathcal{W} of opposite signs in the forward process. In particular, it states that the probability that \mathcal{W}/T takes values opposite to the most probable ones around w_0 is suppressed by the exponential factor $e^{-T w_0}$ for large times T .

Recall from the definition (8.2) that \mathcal{W} differs from the extensive quantity $\int_0^T \mathcal{J}_t dt$ by a boundary term which should not contribute to the large deviations if φ_T stays bounded, although the presence of such terms may change the time-scales on which the large deviation regime is effectively visible. On the contrary, unbounded φ_T may give contributions to the large deviations statistics [83, 9, 86, 70]. For the deterministic dynamics where $\int_0^T \mathcal{J}_t dt = -\int_0^T (\nabla \cdot u)(\mathbf{x}_t) dt$ is the phase-space contraction along the trajectory, see Eq. (8.11), the identity (15.2) with $\zeta' = \zeta$ is essentially the original Gallavotti-Cohen fluctuation relation [35, 31] established rigorously by the authors for the reversible Anosov dynamical systems with discrete time. For such systems, the thermodynamic formalism [75, 34] may be used to prove the existence of the stationary (SRB) measure and of the large deviations regime for the phase-space contraction, see also [74] for a somewhat different approach. In [56], the fluctuation relation (15.2) was discussed for the Langevin-Kramers dynamics, see also [59, 57]. Its version considered here for a general stationary diffusion process is equivalent in the case of vanishing time-inversion-odd drift u_- to the fluctuation relation discussed in [59], see Eq. (5.8) therein.

As another (although related) example of how the transient fluctuation relations yield stationary ones involving large deviations, let us recall the case of the tangent process in the homogeneous Kraichnan model leading to the Itô multiplicative SDE (7.8) (or the Stratonovich SDE (7.10) equivalent to it) and defining the matrix-valued process \mathbf{X}_t .

We have established for it the transient fluctuation relation (7.12) that may be rewritten as the identity

$$E_1^0 \det(X_T) f(X_T) = E_1^0 f(X_T^{-1}) \quad (15.3)$$

for functions f of real $d \times d$ matrices with positive determinant. Such matrices X may be cast into the form

$$X = O' \text{diag}(e^{\rho_1}, \dots, e^{\rho_d}) O^{-1} \quad (15.4)$$

with a diagonal matrix of non-increasing positive entries sandwiched between two orthogonal ones. Note that $\ln \det X = \sum \rho_i$. The so called **stretching exponents** $\rho_1 \geq \dots \geq \rho_d$ are uniquely defined by Eq.(15.4). Consider functions $f(X)$ that are left- and right-invariant under the action of the orthogonal group $O(d)$. They may be viewed as functions of the vector $\vec{\rho}$ of the stretching exponents. The distribution $P_T(d\vec{\rho})$ of such exponents is defined by the relation

$$E_1^0 f(X_T) = \int_{\vec{\rho}_1 \geq \dots \geq \vec{\rho}_d} f(\vec{\rho}) P_T(d\vec{\rho}).$$

The identity (15.3) implies then that

$$P_T(d\vec{\rho}) e^{\sum \vec{\rho}_i} = P_T(d(-\vec{\rho})), \quad (15.5)$$

where $-\vec{\rho} = (-\rho_d, \dots, -\rho_1)$ is the vector of the stretching exponents of the matrix X^{-1} . In a few particular situations (e.g. in the isotropic case), it has been established that for long times and $\vec{\rho}/T = \mathcal{O}(1)$, the distribution of the stretching exponents takes the large deviation form

$$P_T(d\vec{\rho}) \propto e^{-T Z(\vec{\rho}/T)} d\vec{\rho}$$

and the identity (15.5) implies then the stationary fluctuation relation

$$Z(\vec{\sigma}) - \sum_{i=1}^d \sigma_i = Z(-\vec{\sigma}), \quad (15.6)$$

see [11]. Since $-\sum \rho_i$ represents the phase-space contraction $-\ln \det X_t$ in the Kraichnan model, the relation (15.6) may be viewed as a modified Gallavotti-Cohen identity (15.2) for the homogeneous Kraichnan model. The modification goes in two directions. On one hand, the original Gallavotti-Cohen relation involved the deterministic dynamics, whereas the relation (15.6) pertains to random Kraichnan dynamics. On the other hand, it refers to the “multiplicative” large deviations for the vector $\vec{\rho}$ of the stretching exponents containing more detailed information than the phase-space contraction represented by $-\sum \rho_i$. For example, the most probable values of the **stretching rates** $\sigma_i = \rho_i/T$ for which $Z(\vec{\sigma}) = 0$ define the **Lyapunov exponents** λ_i whereas the most probable phase-space contraction rate is equal to the negative of their sum. We shall see in the next section how to extend such multiplicative fluctuation relations to the general diffusive processes. The source of such an extension resides in transient relations that may be proven for general random or deterministic dynamical systems by a simple change-of-variables argument *à la* Evans-Searles [26], as first indicated in [1].

16. Multiplicative Fluctuation Relations

As we have mentioned above, the SDE (2.1) defining the diffusive process \mathbf{x}_t may be used to induce other diffusive processes, the simplest example being the tangent process $(\mathbf{x}_t, \mathbf{X}_t)$ introduced in Sect. 4 and satisfying the SDEs

$$\dot{\mathbf{x}} = u_t(\mathbf{x}) + v_t(\mathbf{x}), \quad \dot{\mathbf{X}} = U_t(\mathbf{x}, \mathbf{X}) + V_t(\mathbf{x}, \mathbf{X})$$

with

$$U_t^i{}_j(\mathbf{x}, \mathbf{X}) = (\partial_k u_t^i)(\mathbf{x}) X^k{}_j, \quad V_t^i{}_j(\mathbf{x}, \mathbf{X}) = (\partial_k v_t^i)(\mathbf{x}) X^k{}_j,$$

see Eq. (4.2). The covariance of the white noise vector field (v_t, V_t) is given by the relations (2.2) and

$$\begin{aligned} \langle v_t^i(\mathbf{x}) V_s^k{}_l(\mathbf{y}, Y) \rangle &= \delta(t-s) \partial_{y^m} D_t^{ik}(\mathbf{x}, \mathbf{y}) Y^m{}_l, \\ \langle V_t^p{}_r(\mathbf{x}, X) v_s^j(\mathbf{y}) \rangle &= \delta(t-s) \partial_{x^n} D_t^{pj}(\mathbf{x}, \mathbf{y}) X^n{}_r, \\ \langle V_t^p{}_r(\mathbf{x}, X) V_s^k{}_l(\mathbf{y}, Y) \rangle &= \delta(t-s) \partial_{x^n} \partial_{y^m} D_t^{pk}(\mathbf{x}, \mathbf{y}) X^n{}_r Y^m{}_l. \end{aligned}$$

One may now apply the theory developed above for general diffusion processes to the case of the tangent process. As an example, let us consider the natural time inversion of Sect. 6.1 corresponding to the trivial splitting

$$(u_{t,+}, U_{t,+}) = 0, \quad (u_{t,-}, U_{t,-}) = (u_t, U_t)$$

and to the involution

$$(\mathbf{x}, \mathbf{X})^* = (\mathbf{x}^*, \mathbf{X}^*) \quad \text{with} \quad (X^*)^i{}_j = (\partial_k x^{*i})(\mathbf{x}) X^k{}_j.$$

The backward process $(\mathbf{x}'_t, \mathbf{X}'_t)$ satisfies in this case the SDE

$$\dot{\mathbf{x}}' = u'_t(\mathbf{x}') + v'_t(\mathbf{x}'), \quad \dot{\mathbf{X}}' = U'_t(\mathbf{x}', \mathbf{X}') + V'_t(\mathbf{x}', \mathbf{X}')$$

with

$$\begin{aligned} u_t^i(\mathbf{x}) &= -(\partial_k x^{*i})(\mathbf{x}^*) u_{t^*}^k(\mathbf{x}^*), \\ U'_t(\mathbf{x}, \mathbf{X}) &= -(\partial_k \partial_m x^{*i})(\mathbf{x}^*) (X^*)^m{}_j u_{t^*}^k(\mathbf{x}^*) - (\partial_m x^{*i})(\mathbf{x}^*) U_{t^*}^m{}_j(\mathbf{x}^*, \mathbf{X}^*) \\ &= (\partial_n u_t^i)(\mathbf{x}) X^n{}_j \end{aligned}$$

and, similarly,

$$v_t^i(\mathbf{x}) = \pm (\partial_k x^{*i})(\mathbf{x}^*) v_{t^*}^k(\mathbf{x}^*), \quad V'_t(\mathbf{x}, \mathbf{X}) = (\partial_n v_t^i)(\mathbf{x}) X^n{}_j.$$

Note that the backward process $(\mathbf{x}'_t, \mathbf{X}'_t)$ defined this way coincides with the tangent process of \mathbf{x}'_t . Equations. (3.4) applied to case at hand give:

$$\begin{aligned} (\hat{u}_{t,+}^i(\mathbf{x}), (\hat{U}_{t,+})^k{}_l(\mathbf{x}, \mathbf{X})) &= -\frac{d+1}{2} (\partial_{y^n} D^{in}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}, \partial_{x^n} \partial_{y^m} D^{km}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}} X^n{}_l) \\ &= -\frac{d+1}{2} (0, (X^{-1})^r{}_p) \begin{pmatrix} d_t^{ij}(\mathbf{x}) & \partial_{y^m} D_t^{ik}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}} X^m{}_l \\ \partial_{x^n} D_t^{pj}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}} X^n{}_r & \partial_{x^n} \partial_{y^m} D_t^{pk}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}} X^n{}_r X^m{}_l \end{pmatrix} \end{aligned}$$

in the matrix notation, where the matrix on the right hand side is the counterpart of $(d_t^{ij}(x))$ for the tangent process. Substituting the above expression to the definition (7.6), we infer that

$$\begin{aligned} \mathcal{J}_t &= -(d+1)(X_t^{-1})^r_p \dot{X}_t^p_r + (d+1)(X_t^{-1})^r_p \partial_n u_t^p(\mathbf{x}_t) X_t^n_r - (d+1) \partial_n u_t^n(\mathbf{x}_t) \\ &= -(d+1) \frac{d}{dt} \ln \det X_t. \end{aligned}$$

The relation (7.7) of Sect. 7 gives then for the case of the tangent process the identity

$$\begin{aligned} dx dX_0 P_{0,T}(x, X_0; dy, dX) (\det X_0)^{-(d+1)} (\det X)^{d+1} \\ = dy dX P'_{0,T}(y^*, X^*; dx^*, dX_0^*) \end{aligned}$$

that may be viewed as an extension of the relation (7.11) obtained in Example 5 for the homogeneous Kraichnan process to a general diffusive process. Similarly as in Example 5, we infer from the above equation the **multiplicative fluctuation relation**

$$dx P_{0,T}(x, 1; dy, dX) (\det X) = dy P'_{0,T}(y^*, 1^*; dx^*, d(X^{-1})^*). \quad (16.1)$$

Suppose that we are given a Riemannian metric γ on \mathbf{R}^d (for example the usual flat one). Since the matrix $X = X_T$ maps the tangent space at $x = \mathbf{x}_0$ to the one at $y = \mathbf{x}_T$, see Eq. (4.2), it is natural to define the stretching exponents $\vec{\rho}$ of X by the relation (15.4) with O and O' mapping the canonical basis of \mathbf{R}^d into a basis orthonormal with respect to the metric $\gamma(x)$ and $\gamma(y)$, respectively. The joint probability distribution $P_{0,T}(x, dy, d\vec{\rho})$ of the end-point of the process \mathbf{x}_t and of the stretching exponents of X_t is then given by the relation

$$\int f(X) P_{0,T}(x, 1, dy, dX) = \int_{\rho_1 \geq \dots \geq \rho_d} f(\vec{\rho}) P_{0,T}(x, dy, d\vec{\rho})$$

for functions $f(X)$ left- and right-invariant under the action of the orthogonal groups preserving, respectively, the metric $\gamma(x)$ and $\gamma(y)$. Similarly we introduce the kernels $P'_{0,T}(x', dy', d\vec{\rho}')$ using the transition probabilities of the backward process and the metric γ' obtained from γ by the involution $x \mapsto x^*$. Equation (16.1) implies then the identity

$$v_\gamma(dx) P_{0,T}(x, dy; d\vec{\rho}) e^{\sum_i \rho_i} = v_{\gamma'}(dy) P'_{0,T}(y, dx^*; d(-\vec{\rho})),$$

where $v_\gamma(dx)$ is the metric volume measure. For the stationary dynamics, we may expect the emergence of the large deviations regime for the stretching rates with

$$P_{0,T}(x, dy; d\vec{\rho}) \cong e^{-T Z(\vec{\rho}/T)} dy d\vec{\rho}$$

for large T and $\vec{\rho}/T = \mathcal{O}(1)$, and similarly for the backward process. One obtains then the identity

$$Z(\vec{\sigma}) - \sum_{i=1}^d \sigma_i = Z'(-\vec{\sigma}). \quad (16.2)$$

As usually, the rate function Z' for the backward process may be replaced by Z for a time-reversible dynamics. The relation (16.2) generalizes the fluctuation relation (15.6) obtained for the Lagrangian flow in the homogeneous Kraichnan model that was time-reversible. The multiplicative fluctuation relations were studied recently in [30] also for particles with inertia carried by the homogeneous Kraichnan flow. Due to the Stokes friction force, the standard time-reversibility is broken in such a system, leading to a modification of the relation between the rate functions Z' and Z .

17. Towards N -Point Hierarchy of Fluctuation Relations

Another way to induce new diffusive processes from the original one described by the SDE (2.1) is to consider simultaneously its N solutions starting at different initial points. They may be viewed as a solution of the SDE

$$\dot{\mathbf{x}} = \mathbf{u}_t(\mathbf{x}) + \mathbf{v}_t(\mathbf{x}) \quad (17.1)$$

with $\mathbf{x} = (x_1, \dots, x_N)$, $\mathbf{u}_t(\mathbf{x}) = (u_t(x_1), \dots, u_t(x_N))$, and $\mathbf{v}_t(\mathbf{x}) = (v_t(x_1), \dots, v_t(x_N))$. The covariance of the white noise vector field $\mathbf{v}_t \equiv (v_{t,1}, \dots, v_{t,N})$ appearing on the right hand side is

$$\langle v_{t,m}^i(\mathbf{x}) v_{s,n}^j(\mathbf{y}) \rangle = \delta(t-s) D_t^{ij}(x_m, y_n).$$

The spatial part of the covariance restricted to the diagonal is

$$d_{t,mn}^{ij}(\mathbf{x}) = D_t^{ij}(x_m, x_n).$$

The machinery producing the fluctuation relations described in this paper may be applied to the N -point diffusion process governed by the SDE (17.1), at least if the matrix $(d_{t,mn}^{ij}(\mathbf{x}))$ is invertible, recall that the inverse of the matrix $(d_t^{ij}(x))$ appears in the expression (7.6) for \mathcal{J}_t . We postpone a closer examination of the possible hierarchy of fluctuation relations obtained this way to the future. Here, let us only remark that the tangent process $(\mathbf{x}_t, \mathbf{X}_t)$, which was studied in the preceding section and led to the multiplicative fluctuation relation (16.1), could be viewed as a limiting case of the $(d+1)$ -point process where the last d points are infinitesimally close to the first one.

18. Conclusions

We have developed a unified approach to fluctuation relations for finite-dimensional diffusion processes. The setup of the paper covered the cases of deterministic dissipative continuous-time dynamical systems, of the Langevin dynamics with non-conservative forces, and of the Kraichnan model of hydrodynamic flows. The fluctuation relations were obtained by comparing the forward diffusion process to the backward one produced by a time inversion. We have admitted different time inversions that treated differently two parts of the deterministic drift in the diffusion equations. This was physically motivated in situations when one part of the drift was assimilated with a dissipative and another one with a conservative force, but was used in other situations as well, leading to a greater flexibility. As particular cases, we discussed the natural time inversion used for deterministic systems, its slight modification for stochastic dynamics that permitted to take easily the deterministic limit of fluctuation relations, as well as the reverse

protocol and the current reversal discussed in a similar context in [10], and the complete reversal. We showed that any of the allowed time inversions leads to a detailed fluctuation relation (13.3) of Proposition 7 that may be viewed as a constrained version of the generalized detailed balance relation to which the identity (13.3) reduces in the case of the complete reversal. The constraint fixes the value of the entropy production measured relative to the corresponding backward process. We obtained various transient fluctuation relations as corollaries of the detailed one. Among examples were the Evans-Searles fluctuation relation (14.1), the Crooks one (13.5), and various versions of the Jarzynski equality (8.7), including the original ones for the deterministic Hamiltonian dynamics and for the Langevin dynamics with local detailed balance (8.9), the one for reversed protocol, and the Hatano-Sasa one. By comparing the detailed fluctuation relations for two different time inversions, we obtained also a generalization (9.2) of the Speck-Seifert equality (9.5). For the sake of completeness, we included into the paper a derivation from the Jarzynski equality of the Green-Kubo and the Onsager relations, and of the fluctuation-dissipation theorem. On a simple example of a one-dimensional Langevin equation with spontaneously broken equilibrium, we indicated how in such a situation the Hatano-Sasa version of the Jarzynski equality induced corrections to the fluctuation-dissipation theorem proportional to the flux of the probability current.

In the case of stationary diffusion processes, we pointed out that the transient fluctuation relations may give rise to the asymptotic symmetries of the large-deviations rate function of the entropy production which were established first by Gallavotti-Cohen for the uniformly hyperbolic dynamical systems and were extended later to (some) diffusion processes by Kurchan and Lebowitz-Spohn. Finally, we wrote explicitly a detailed fluctuation relation for the induced tangent diffusion process obtained from the original one. This produced a multiplicative transient fluctuation relation that led for long times to a Gallavotti-Cohen-type symmetry of the large-deviations rate function for the stretching exponents governing the behavior of infinitesimally close trajectories of the diffusion process. We speculated that considering distant multi-point trajectories of the process should give rise to a hierarchy of fluctuation relations. It could also provide a way to produce fluctuation relations for flow processes describing the simultaneous evolution of all trajectories of the process [55]. A similar extension should also permit to formulate fluctuation relations for hydrodynamic flows modeling fully developed turbulence [40,60]. We postpone such questions to further studies.

Appendix A.

The Stratonovich SDE (2.1) defining the process \mathbf{x}_t is equivalent to the Itô SDE

$$dx^i = (u_t^i(x) + \tilde{u}_t^i(x)) dt + v_t^i(x) dt ,$$

with the correction term

$$\tilde{u}_t^i(x) = \frac{1}{2} \partial_{x^j} D_t^{ij}(x, y)|_{y=x} .$$

By the Itô calculus, $g(\mathbf{x}_t)$ satisfies the Itô SDE

$$dg(x) = (u_t^i(x) + \tilde{u}_t^i(x)) \partial_i g(x) dt + v_t^i(x) \partial_i g(x) dt + \frac{1}{2} d_t^{ij}(x) \partial_i \partial_j g(x) dt$$

with the second order Itô term. For the expectation of $g(\mathbf{x}_t)$, this gives the ODE

$$\frac{d}{dt} E_x^{t_0} g(\mathbf{x}_t) = E_x^{t_0} (u_t^i(\mathbf{x}_t) + \tilde{u}_t^i(\mathbf{x}_t)) \partial_i g(\mathbf{x}_t) + \frac{1}{2} d_t^{ij}(\mathbf{x}_t) \partial_i \partial_j g(\mathbf{x}_t)$$

from which the formula

$$L_t = (u_t^i + \tilde{u}_t^i(\mathbf{x}_t))\partial_i + \frac{1}{2}d_t^{ij}\partial_i\partial_j,$$

easily seen to be equivalent to Eq. (3.3), follows.

Appendix B.

Proof of Lemma 1.

$$\begin{aligned} (L_{t,-}Rg)(x) &= u_{t,-}^i(x)\partial_i(Rg)(x) = u_{t,-}^i(x)(\partial_i x^{*k})(x)(\partial_k g)(x^*) \\ &= -(u_{t^*,-}^{ik}\partial_k g)(x^*) = -(R L_{t^*,-}'g)(x), \\ (L_{t,+}Rg)(x) &= \hat{u}_{t,+}^i(x)\partial_i(Rg)(x) + \frac{1}{2}\partial_j d_t^{ij}(x)\partial_i(Rg)(x) \\ &= u_{t,+}^i(x)(\partial_i x^{*k})(x)(\partial_k g)(x^*) - \frac{1}{2}\partial_{y^j} D^{ij}(x, y)|_{y=x}(\partial_i x^{*k})(x)(\partial_k g)(x^*) \\ &\quad + \frac{1}{2}(\partial_j x^{*l})(x)\partial_{x^{*l}} d_t^{ij}(x)(\partial_i x^{*k})(x)(\partial_k g)(x^*) \\ &= (u_{t^*,+}^{ik}\partial_k g)(x^*) - \frac{1}{2}(\partial_j x^{*l})(y)\partial_{y^{*l}} D^{ij}(x, y)|_{y=x}(\partial_i x^{*k})(x)(\partial_k g)(x^*) \\ &\quad - \frac{1}{2}(\partial_{x^{*l}}\partial_j x^{*l})(x)d_t^{ij}(x)(\partial_i x^{*k})(x)(\partial_k g)(x^*) \\ &\quad + \frac{1}{2}\partial_{x^{*l}}(\partial_j x^{*l})(x)d_t^{ij}(x)(\partial_i x^{*k})(x)(\partial_k g)(x^*) \\ &= (u_{t^*,+}^{ik}\partial_k g)(x^*) - \frac{1}{2}\partial_{y^{*l}}(\partial_j x^{*l})(y)D_t^{ij}(x, y)(\partial_i x^{*k})(x)|_{y=x}(\partial_k g)(x^*) \\ &\quad + \frac{1}{2}\partial_{x^{*l}}d_t^{ikl}(x^*)(\partial_k g)(x^*) \\ &= (\hat{u}_{t^*,+}^{ik}\partial_k g)(x^*) + \frac{1}{2}(\partial_l d_t^{ikl}\partial_k g)(x^*) = (R L_{t^*,+}'g)(x), \end{aligned}$$

where we have used the relations (3.4), (5.5), (5.6) and (5.7). \square

Appendix C.

In order to prove the first of the equalities (6.2), let us note that the condition $\hat{u}_{t,+} = 0$ means that

$$u_{t,+}^i(x) = \frac{1}{2}\partial_{y^j} D_t^{ij}(x, y)|_{y=x}$$

so that, according to Eqs. (5.5) and (5.6),

$$\begin{aligned} u_{t^*,+}^i(x^*) &= (\partial_k x^{*i})(x)\frac{1}{2}\partial_{y^l} D_t^{kl}(x, y)|_{y=x} \\ &= \frac{1}{2}\partial_{y^n}(\partial_j x^{*n})(y^*)(\partial_l x^{*j})(y)(\partial_k x^{*i})(x)D_t^{kl}(x, y)|_{y=x} \\ &= \frac{1}{2}(\partial_j x^{*n})(y^*)\partial_{y^n}(\partial_k x^{*i})(x)D_t^{kl}(x, y)(\partial_l x^{*j})(y)|_{y=x} \\ &\quad + \frac{1}{2}(\partial_{y^n}(\partial_j x^{*n})(x^*))(\partial_k x^{*i})(x)d_t^{kl}(x)(\partial_l x^{*j})(x) \\ &= \frac{1}{2}\partial_{y^j} D_t^{ij}(x^*, y)|_{y=x^*} + \frac{1}{2}(\partial_n x^{*k})(x)(\partial_k \partial_j x^{*n})(x^*)d_t^{ij}(x^*) \\ &= \frac{1}{2}\partial_{y^j} D_t^{ij}(x^*, y)|_{y=x^*} + \frac{1}{2}d_t^{ij}(x^*)(\partial_j \ln \sigma)(x^*), \end{aligned}$$

where we used the identity

$$(\partial_j \ln \sigma)(x^*) = (\partial_n x^{*k})(x)(\partial_j \partial_k x^{*n})(x^*)$$

to obtain the last equality. The first of the relations in Eqs. (6.2) follows. The second one is an immediate consequence of the transformation rule in Eqs. (5.5).

Appendix D.

Proof of Lemma 2. The Cameron-Martin-Girsanov formula⁵ says that if y_t is the diffusion process solving the SDE

$$\dot{y} = w_t(y) + u_t(y) + v_t(y), \quad (\text{D.1})$$

then

$$E_x^{t_0} \mathcal{F}(y) = E_x^{t_0} \mathcal{F}(x) e^{-U(x)}$$

for x_t solving the SDE (2.1) and

$$\begin{aligned} U(x) = & \int_{t_0}^t \left[-w_s(x_s) \cdot d_s^{-1}(x_s) \dot{x}_s + w_s(x_s) \cdot d_s^{-1}(x_s) \hat{u}_s(x_s) \right. \\ & \left. + \frac{1}{2} w_s(x_s) \cdot d_s^{-1}(x_s) w_s(x_s) + \frac{1}{2} (\nabla \cdot w_s)(x_s) \right] ds \end{aligned}$$

if the functional \mathcal{F} depends on the process restricted to the time interval $[t_0, t]$. The first term under the integral in the expression for $U(x)$ has to be interpreted with the Stratonovich rule. Denoting by \tilde{L}_t the generator of the process y_t solving the SDE (D.1),

$$\tilde{L}_t = (w_t^i + \hat{u}_t^i) \partial_i + \frac{1}{2} \partial_j d_t^{ij} \partial_i,$$

we obtain this way the relation

$$\begin{aligned} \tilde{P}_{t_0, t}(x, dy) & \equiv E_x^{t_0} \delta(y_t - y) dy = \overrightarrow{\mathcal{T}} \exp \left[\int_{t_0}^t \tilde{L}_s ds \right] (x, dy) \\ & = E_x^{t_0} e^{-U(x)} \delta(x_t - y) dy. \end{aligned}$$

Next, if $f_t(x)$ is a time-dependent function then, by the Feynman-Kac formula,

$$\overrightarrow{\mathcal{T}} \exp \left[\int_{t_0}^t (\tilde{L}_s - f_s) ds \right] (x, dy) = E_x^{t_0} e^{-U(x) - \int_{t_0}^t f_s(x_s) ds} \delta(x_t - y) dy.$$

The application of the latter formula for $w_t = -2\hat{u}_{t,+}$ and $f_t = -\nabla \cdot \hat{u}_{t,+} + \nabla \cdot u_{t,-}$ gives Eq. (7.5) in view of the relation (7.1). \square

⁵ We have transformed the formula usually written in the Itô convention [79] to the Stratonovich one.

Appendix E.

Here we show that the matrix M given by Eq.(7.29), where Γ and C are strictly positive and Π is antisymmetric, has eigenvalues with negative real parts and that the matrix C may be recovered from Eq.(7.25) by setting $t = \infty$. If λ is an eigenvalue of M , i.e. if

$$-(\Gamma - \Pi)C^{-1}x_\lambda = \lambda x_\lambda$$

for some $x_\lambda \neq 0$ then

$$\lambda = \frac{-x_\lambda \cdot C^{-1}(\Gamma - \Pi)C^{-1}x_\lambda}{x_\lambda \cdot C^{-1}x_\lambda} = \frac{-x_\lambda \cdot C^{-1}\Gamma C^{-1}x_\lambda}{x_\lambda \cdot C^{-1}x_\lambda} < 0.$$

Equation (7.29) implies that

$$MC + CM^T = -2\Gamma$$

which is solved by C_∞ given by Eq.(7.25) with $t = \infty$. Besides, this is the unique solution because if $MD + DM^T = 0$ then

$$\frac{d}{dt} e^{tM} D e^{tM^T} = 0$$

and

$$D = \lim_{t \rightarrow \infty} e^{tM} D e^{tM^T} = 0.$$

Appendix F.

Proof of Proposition 2. It is enough to check the last identity for the so called cylindrical functionals

$$\mathcal{F}(\mathbf{x}) = f(\mathbf{x}_{t_1}, \dots, \mathbf{x}_{t_n})$$

for $0 \leq t_1 \leq \dots \leq t_n \leq T$. Since

$$e^{-\mathcal{W}} = e^{\varphi_0(\mathbf{x}_0)} e^{-\int_0^{t_1} \mathcal{J}_s ds} e^{-\int_{t_1}^{t_2} \mathcal{J}_s ds} \dots e^{-\int_{t_n}^T \mathcal{J}_s ds} e^{-\varphi_T(\mathbf{x}_T)},$$

then, by virtue of Eq. (7.5), the left hand side of Eq.(8.3) is equal to

$$dx \int f(x_1, \dots, x_n) P_{0,t_1}^1(x, dx_1) P_{t_1,t_2}^1(x_1, dx_2) \dots P_{t_n,T}^1(x_n, dy) e^{-\varphi_T(y)}$$

with the integral over x_1, \dots, x_n . With the use of relation (7.4), this may be rewritten as

$$e^{-\varphi_T(y)} dy \int f(x_1, \dots, x_n) P'_{0,t_n^*}(y^*, dx_n^*) \dots P'_{t_2^*,t_1^*}(x_2^*, dx_1^*) P'_{t_1^*,T}(x_1^*, dx^*)$$

and, after the change of variables $x_{i+1}^* \mapsto x'_{n-i}$, as

$$e^{-\varphi_T(y)} dy \int f(x_n'^*, \dots, x_1'^*) P'_{0,t_n^*}(y^*, dx_1') \dots P'_{t_2^*,t_1^*}(x_{n-1}', dx_n') P'_{t_1^*,T}(x_n', dx^*).$$

This is equal to the left hand side of the identity (8.3) since $e^{-\varphi_T(y)} dy = e^{-\varphi'_0(y^*)} dy^*$.

□

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