Inflow rate, a time-symmetric observable obeying fluctuation relations

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While entropy changes are the usual subject of fluctuation theorems, we seek fluctuation relations involving time-symmetric quantities, namely observables that do not change sign if the trajectories are observed backward in time. We find detailed and integral fluctuation relations for the (time integrated) difference between entrance rate and escape rate in mesoscopic jump systems. Such inflow rate, which is even under time reversal, represents the discrete-state equivalent of the phase space contraction rate. Indeed, it becomes minus the divergence of forces in the continuum limit to overdamped diffusion. This establishes a formal connection between reversible deterministic systems and irreversible stochastic ones, confirming that fluctuation theorems are largely independent of the details of the underling dynamics.

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I. INTRODUCTION

The past two decades were characterized by the discussion of fluctuation relations (FRs), or fluctuation theorems, valid for systems arbitrarily far from equilibrium conditions [1–21] (the literature on FRs is vast, see more references in the reviews [22–25]). Initially the focus was on deterministic dynamical systems, where Lyapunov exponents were found to play a fundamental role [1–4]. Although quantities as the phase space contraction rate (minus sum of all Lyapunov exponents) are related to the entropy production [23], this concept acquires a more immediate physical interpretation in terms of heat flows when stochastic systems are considered [6–12, 18–21, 25]. For this reason, and because of the relevance for modern technological applications, nowadays it is more frequent to discuss FRs for stochastic dynamics.

The production of entropy, $S(\omega)$, being related to fluxes of heat, matter, etc., changes sign if one goes through the trajectory ω backward in time. By now it is essentially understood that any FR under examination involves a form of entropy production, and that it yields a measure of the statistical asymmetry of physical processes in time. For example, the integral FR $\langle e^{-S} \rangle = 1$ $\langle \ldots \rangle$ denotes a statistical average) and the convexity of the exponential function provide a statistical mechanical derivation of the second law of thermodynamics, $\langle S \rangle \geq 0$. Such asymmetry in time exists already at the level of trajectories. Entropy production is the physical quantity that always determines the time-antisymmetric sector of path probabilities [12, 25],

$$P(\omega) \sim e^{-\mathcal{A}(\omega)} \sim e^{\frac{1}{2}[S(\omega) - K(\omega)]},$$
 (1)

which is generally written as an exponential of some functional A. This includes also a time symmetric (TS) com-

ponent $K(\omega)$. Yet, such a quantity is completely irrelevant in the standard procedure used to prove FRs, in which one compares path weights (1) with those of trajectories reversed in time.

However, it is important to sharpen our understating of the meaning and the statistics of TS quantities, since it is becoming clear that they are necessary in the formulation of nonequilibrium statistical mechanics. A TS quantity that was recognized as a major player in characterizing the evolution of glassy systems is dynamical activity [26–33], which is just the number of jumps (or changes of state) that take place during a trajectory, regardless of their direction. Moreover, in the context of linear response theory, one finds fluctuation-dissipation relations where $K(\omega)$ complement the entropy production in determining the response of systems far from equilibrium [34–38]. Mostly these TS observables were continued to be called dynamical activity, although sometimes also the names "traffic" [39] or "frenesy" [36] were adopted. There are few examples of fluctuation symmetries for TS quantities [28, 33]. Therefore, to better understand the physics of nonequilibrium systems, there remains the interest of going deeper in this direction and find more variants of FRs for TS observables.

In this paper we briefly introduce some FRs for TS quantities. In discrete jump processes we study the *inflow rate* in a state, expressed as a properly defined entrance rate minus the standard escape rate. The derivation of FRs is based on an artificial "auxiliary" dynamics. A similar idea was recently put forward [21] to define the path-space probability of trajectories reversed in time when some transitions are only one way (i.e. their reverse transition does not exists). With such an approach one may draw a generalized FR [21]. By taking this method to the extreme, we will define the auxiliary dynamics as that taking place when all jump rates are flipped. It is a simple mathematical choice that leads to specific FRs. The probability of the auxiliary dynamics, appearing in such FRs, can be traced out and one is left with inte-

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gral FRs, valid for the normal dynamics and in terms of sound physical quantities.

When we perform the limit to overdamped diffusive dynamics, we make contact with the approach by Maes and van Wieren [28]: the auxiliary dynamics here corresponds to flipping the force signs and the inflow rate becomes minus the divergence of the forces, which is the phase space contraction rate of the associated noiseless dynamics. In our case the contraction rate is even under time reversal, differently from the case of reversible deterministic dynamical systems. Nevertheless, an integral fluctuation for this quantity is derived. Note that the contraction rate can be found, for conservative forces, within the definition of the so-called effective potential, which is used in computations of reaction pathways [40] and in evaluations of the system activity [41, 42].

II. JUMP PROCESS

We consider a system with discrete states $\{C\}$ whose probabilities ρ_t evolve according to the master equation

$$\partial_t \rho_t(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} \left[\rho_t(\mathcal{C}') k(\mathcal{C}' \to \mathcal{C}) - \rho_t(\mathcal{C}) k(\mathcal{C} \to \mathcal{C}') \right], \quad (2)$$

where $k(\mathcal{C} \to \mathcal{C}')$ is the transition rate from configuration \mathcal{C} to \mathcal{C}' . The last term in the master equation contains the probability $\rho_t(\mathcal{C})$ times the escape rate from \mathcal{C}

$$\lambda(\mathcal{C}) \equiv \sum_{\mathcal{C}' \neq \mathcal{C}} k(\mathcal{C} \to \mathcal{C}'). \tag{3}$$

Here, next to this concept, we find it useful to define the entrance rate $\varepsilon(\mathcal{C})$ as the sum of transition rates from \mathcal{C}' to \mathcal{C} ,

$$\varepsilon(\mathcal{C}) \equiv \sum_{\mathcal{C}' \neq \mathcal{C}} k(\mathcal{C}' \to \mathcal{C}).$$
 (4)

In physics often one considers transition rates obeying local detailed balance [43] at temperature $T = 1/\beta$,

$$k(\mathcal{C} \to \mathcal{C}') \sim \exp\left[\frac{\beta}{2}\mathcal{W}(\mathcal{C} \to \mathcal{C}')\right]$$
 (5)

where $\mathcal{W}(\mathcal{C} \to \mathcal{C}')$ is the work done by the system on its environment (a heat bath in equilibrium). The term $\beta \mathcal{W}(\mathcal{C} \to \mathcal{C}')$ thus represents the increase of entropy in the environment associated to the jump $\mathcal{C} \to \mathcal{C}'$ in the system.

A trajectory from time $t_0 = 0$ to time t is the timeordered sequence $\omega \equiv \{\mathcal{C}(s)|0 \leq s \leq t\} = \{\mathcal{C}_0 = \mathcal{C}(0), \mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_n = \mathcal{C}(t)\}$ with n jumps $\mathcal{C}_{i-1} \to \mathcal{C}_i$ taking place at times t_i . For a system with initial density $\rho_0(\mathcal{C})$, the probability to observe a trajectory ω is proportional to

$$P(\omega) \sim \rho_0(\mathcal{C}_0) e^{-\lambda(\mathcal{C}_n)(t-t_n)} \prod_{i=0}^{n-1} k(\mathcal{C}_i \to \mathcal{C}_{i+1}) e^{-\lambda(\mathcal{C}_i)(t_{i+1}-t_i)}$$
$$\sim \rho_0(\mathcal{C}_0) e^{-\int_0^t ds \lambda(\mathcal{C}(s))} \prod_{i=0}^{n-1} k(\mathcal{C}_i \to \mathcal{C}_{i+1})$$
(6)

(we are omitting a time-discretization prefactor that is common to all trajectories with the same number of jumps [44]). The standard FR of the entropy production is obtained already at the level of single trajectories by comparing $P(\omega)$ with the probability of the path reversed in time, which we obtain by applying an involution θ that reverses the order of times ($\theta\omega \equiv \{\mathcal{C}(t-s)|0 \leq s \leq t\}$, i.e. the initial time of $\theta\omega$ is what it was the final time for ω , etc.). Thus,

$$\frac{P(\omega)}{P(\theta\omega)} = e^{S_{\text{tot}}(\omega)},\tag{7}$$

with

$$S_{\text{tot}}(\omega) = -\ln \rho_t(\mathcal{C}_n) + \ln \rho_0(\mathcal{C}_0) + \beta \sum_{i=0}^{n-1} \mathcal{W}(\mathcal{C}_i \to \mathcal{C}_{i+1})$$
$$= -\ln \rho_t(\mathcal{C}_n) + \ln \rho_0(\mathcal{C}_0) + S(\omega), \tag{8}$$

where $S(\omega)$ is the entropy increase in the heat bath. From (7) one readily observes that an increase of the entropy in the bath is associated with processes more likely to take place in the normal direction of time, because typically $\frac{P(\omega)}{P(\theta\omega)} > 1$ in this case (excluding effects from the boundary terms). Note that by construction this equation picks up the time-antisymmetric portion of the path measures and completely forgets about the integral of escape rates.

To obtain a new form of FR we do not simply consider time-reversal but we rather define an auxiliary dynamics where all rates are replaced by the rates of the inverse transitions,

$$k^*(\mathcal{C} \to \mathcal{C}') \equiv k(\mathcal{C}' \to \mathcal{C}),$$
 (9)

so that the "auxiliary" escape rates correspond to the entrance rates of the normal dynamics.

$$\lambda^*(\mathcal{C}) \equiv \sum_{\mathcal{C}' \neq \mathcal{C}} k^*(\mathcal{C} \to \mathcal{C}') = \varepsilon(\mathcal{C}). \tag{10}$$

Note that other choices for "adjoint dinamics" have already been discussed [15–17]. However, those are useful to single out specific entropy production terms only.

The state density ρ^* with the auxiliary dynamics is chosen to be the same ρ we have with the normal dynamics. Thus, the path probability under the auxiliary dynamics is

$$P^*(\omega) \sim \rho_0^*(\mathcal{C}_0) e^{-\int_0^t dt' \lambda^*(t')} \prod_{i=0}^{n-1} k^*(\mathcal{C}_i \to \mathcal{C}_{i+1})$$
$$\sim \rho_0(\mathcal{C}_0) e^{-\int_0^t dt' \varepsilon(t')} \prod_{i=0}^{n-1} k(\mathcal{C}_{i+1} \to \mathcal{C}_i), \quad (11)$$

while for the corresponding time-reversed path it reads

$$P^*(\theta\omega) \sim \rho_t(\mathcal{C}_n) e^{-\int_0^t dt' \varepsilon(t')} \prod_{i=0}^{n-1} k(\mathcal{C}_i \to \mathcal{C}_{i+1}). \tag{12}$$

The initial densities of $P^*(\omega)$ and $P^*(\theta\omega)$ are taken to be the initial and final densities of the physical trajectory, respectively, ρ_0 and ρ_t . Any other choice is equally allowed, though (see Sec. IV).

It is clear that the ratio of the path measure (11) or (12) with (6) now yields the exponential of a novel path-dependent term

$$Y(\omega) = \int_0^t dt' [\varepsilon(\mathcal{C}(t')) - \lambda(\mathcal{C}(t'))]$$

$$\equiv \int_0^t dt' \, \mathcal{R}(\mathcal{C}(t')), \tag{13}$$

in which there plays a crucial role the instantaneous inflow rate, i.e. the imbalance between the entrance rate (4) and the escape rate (3)

$$\mathcal{R}(\mathcal{C}) \equiv \varepsilon(\mathcal{C}) - \lambda(\mathcal{C}). \tag{14}$$

Specifically, the ratio of Eqs. (11) and (6) is

$$\frac{P^*(\omega)}{P(\omega)} = e^{-S(\omega) - Y(\omega)},\tag{15}$$

while the ratio of Eqs. (12) and (6) is

$$\frac{P^*(\theta\omega)}{P(\omega)} = e^{\ln[\rho_t(C_n)/\rho_0(C_0)] - Y(\omega)}.$$
 (16)

Using the fact that $P(\theta\omega)$ can be normalized to 1 $(\int \mathcal{D}\omega P^*(\theta\omega) = 1 = \langle 1 \rangle^*)$ and the conversion of statistical averages $\langle \ldots \rangle^* = \langle \ldots P^*/P \rangle$, from (16) we obtain the integral FR

$$\left\langle e^{\ln[\rho_t(\mathcal{C}_n)/\rho_0(C_0)]-Y(\omega)} \right\rangle = 1,$$
 (17)

which becomes

$$\left\langle e^{-Y(\omega)} \right\rangle \to 1 \quad \text{for } t \to \infty$$
 (18)

if the boundary contribution is irrelevant. This occurs for instance for $t \to \infty$ if the system has a finite number of states and is in a stationary regime, $\rho_t = \rho_0 \,\forall t$. The convexity of the exponential yields also the inequality $\langle Y(\omega) \rangle \geq 0$. A positive inflow rate is to be expected as it is easier on average to jump into the states with high ρ than into those with low ρ .

With a similar procedure but using (15) rather than (16) one obtains another FR

$$\left\langle e^{-Y(\omega)-S(\omega)} \right\rangle = 1,$$
 (19)

where the entropy production S reappears next to Y. Note that (17) and (19) are valid also in transient conditions. An equation as (19) might be particularly interesting in transient regimes because it does not contain explicitly the initial and final density of states. Possibly it might help to study glassy systems, which are the paradigm of transient dynamics.

III. OVERDAMPED DIFFUSION

In order to identify the transformation of a diffusive dynamics equivalent to inverting the rates in a jump process we start from the generic Fokker-Planck equation [45] for the density $\rho_t(x)$,

$$\partial_t \rho_t(x) = -\partial_x (\mu F(x)\rho_t(x)) + D\partial_x^2 \rho_t(x), \tag{20}$$

where μ is a mobility, D is a diffusion constant, and F(x) is a force. We discretize phase space in tiny units of size δ , so (20) turns into a master equation for configurations $C = \ldots, x - \delta, x, x + \delta, \ldots$ With the standard assumption that the dynamics is performed by random walks with jumps to nearest neighbors $x \to y = x \pm \delta$, the discretization yields

$$\partial_t \rho_t(x) = -\frac{\mu}{2\delta} [F(x+\delta)\rho_t(x+\delta) - F(x-\delta)\rho_t(x-\delta)] + \frac{D}{\delta^2} [\rho_t(x+\delta) + \rho_t(x-\delta) - 2\rho_t(x)], \tag{21}$$

that can be rewritten as a master equation with transition rates

$$k(x \to y) = \begin{cases} \frac{D}{\delta^2} - \frac{\mu}{2\delta} F(x - \delta) & \text{if } y = x - \delta \\ \frac{D}{\delta^2} + \frac{\mu}{2\delta} F(x + \delta) & \text{if } y = x + \delta. \end{cases}$$
(22)

When we apply the transformation $k^*(x \to y) = k(y \to x)$ we obtain

$$k^*(x \to y) = \begin{cases} \frac{D}{\delta^2} + \frac{\mu}{2\delta} F(x) & \text{if } y = x - \delta \\ \frac{D}{\delta^2} - \frac{\mu}{2\delta} F(x) & \text{if } y = x + \delta. \end{cases}$$
 (23)

The difference in the state where the forces are evaluated is of order O(1) [46], and so vanishes when we go back to the continuous limit $\delta \to 0$ (D is assumed to be a constant). We conclude that changing the sign of F (or alternatively of μ) gives the transformed rates in terms of the original ones, namely $k_F^*(x \to y) = k_{-F}(x \to y)$. The path weight associated to (20), describing overdamped diffusive dynamics, is

$$P(\omega) \sim \rho_0(x(0)) \exp\left\{-\int_0^t dt' \frac{\left[\dot{x}(t') - \mu F(t')\right]^2}{4D} - \frac{\mu}{2} \int_0^t dt' \partial_x F(t')\right\}$$
(24)

and it is straightforward to obtain the equivalent of (17) by applying time reversal together with the transformation $F^* = -F$ (or equivalently $\mu^* = -\mu$), which again gives the probability ratio

$$\frac{P^*(\theta\omega)}{P(\omega)} = \frac{\rho_t^*(x(t))}{\rho_0(x(0))} e^{-Y(\omega)} = e^{\ln[\rho_t(x(t))/\rho_0(x(0))] - Y(\omega)},$$
(25)

where now the integral Y is

$$Y(\omega) = -\mu \int_0^t dt' \partial_x F(t'). \tag{26}$$

In [28] we found the only previous example where one force was flipped to get a FR for TS quantities. Alternatively, we can get again

$$\frac{P^*(\omega)}{P(\omega)} = e^{-S(\omega) - Y(\omega)},\tag{27}$$

where the entropy increase in the heat bath is here defined by

$$S(\omega) = \frac{\mu}{D} \int_0^t dt' F(t') \dot{x}(t'). \tag{28}$$

Therefore, we find Eqs. (17), (18) and (19) to be valid also in overdamped diffusing systems. Besides, from (25) one can as well derive detailed FRs that link the statistics of observables (odd under the joint inversion of time and forces) in two systems subject to opposite forces. Examples of practical interest are systems of non-interacting particles exposed to controllable external fields.

In more than one dimension and with $\mu=1,$ Eq. (26) reads

$$Y(\omega) = -\int_0^t dt' \partial_{x_i} F_i(\boldsymbol{x}(t')). \qquad (29)$$

Einstein notation is used from here onward and the vector state is denoted as $x \equiv \{x_i\}$. For overdamped stochastic systems the inflow rate is thus represented by a function with the structure of a divergence of forces,

$$\mathcal{R}(\boldsymbol{x}) = -\partial_{x_i} F_i(\boldsymbol{x}) \tag{30}$$

when all mobilities are equal to 1. This form has an analogous version in deterministic evolution, as discussed in the next section.

IV. ANALOGY WITH THE CONTRACTION RATE

Consider a dynamical systems composed of $i=1,\ldots,N$ degrees of freedom evolving according to deterministic equations

$$\dot{x}_i = F_i(\boldsymbol{x}). \tag{31}$$

In phase space the system is described by a density ρ which evolves according to the continuity equation, enforcing probability conservation:

$$\partial_t \rho(\mathbf{x}(t), t) = -\partial_{x_i} [\dot{x}_i(t) \rho(\mathbf{x}(t), t)]$$

= $-\partial_{x_i} [F_i(\mathbf{x}(t)) \rho(\mathbf{x}(t), t)].$ (32)

Rearranging the terms and introducing the Lagrangian derivative $d/dt \equiv \partial_t + \dot{x}_i \partial_{x_i}$ accounting for time variations along trajectories, we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\ln\rho(\boldsymbol{x}(t),t) = -\partial_{x_i}F_i(\boldsymbol{x}(t)) \equiv \sigma(\boldsymbol{x}(t)). \tag{33}$$

In (33) we introduced the instantaneous contraction rate $\sigma(\boldsymbol{x})$, which measures the logarithmic rate of contraction of phase space volumes [47] —it is identically zero in Hamiltonian systems and on average positive in dissipative ones [48]. This is exactly the quantity (30) for which we have derived a FR for the diffusive dynamics. Moreover, since the transformation used to find the FR in the discrete dynamics (see Sec. II) is analogous to that used to derive the FR in the diffusive dynamics, we conclude that the inflow rate $\mathcal{R}(\mathcal{C})$ is the equivalent of the contraction rate $\sigma(\boldsymbol{x})$.

There is indeed a procedure that illustrates this correspondence. In a discrete state system, we spread uniformly the occupation probability on the configuration \mathcal{C} and on its neighbors, i.e. those \mathcal{C}' such that $k(\mathcal{C} \to \mathcal{C}') \neq 0$. At t = 0 we thus have $\rho_0(\mathcal{C}) = \rho_0(\mathcal{C}') = 1/\mathcal{V}(\mathcal{C})$, where $\mathcal{V}(\mathcal{C})$ is the number, or "volume", of the states centered around \mathcal{C} . Shortly after the preparation, the time derivative of the Boltzmann entropy associated to this locally flat density is expected to give the logarithmic variation of the inverse volume centered on \mathcal{C} . Therefore we have

$$\partial_{t} \ln \rho_{t}(\mathcal{C}(t))|_{t=0} = \mathcal{V}(\mathcal{C})\partial_{t}\rho_{t}(\mathcal{C})|_{t=0}$$

$$= \mathcal{V}(\mathcal{C}) \sum_{\mathcal{C}'} \left[\rho_{t}(\mathcal{C}')k(\mathcal{C}' \to \mathcal{C}) - \rho_{t}(\mathcal{C})k(\mathcal{C} \to \mathcal{C}')\right]\Big|_{t=0}$$

$$= \sum_{\mathcal{C}'} \left[k(\mathcal{C}' \to \mathcal{C}) - k(\mathcal{C} \to \mathcal{C}')\right]$$

$$= \mathcal{R}(\mathcal{C}), \tag{34}$$

which shows that the inflow rate measures the "volume" contraction rate.

The phase-space contraction rate is a key ingredient in the derivation of FRs for deterministic dynamics [22, 23]. Hence we deem it interesting to strengthen the correspondence between thermostated deterministic systems (i.e., Hamiltonian systems with an added nonlinear friction term) and stochastic ones applying the ideas of Sec. II and Sec. III to underdamped diffusion, where the phase space does not simply reduce to the configuration space. For simplicity we consider two conjugated degrees of freedom only, $\boldsymbol{x} = \{q, mv\}$, exemplifying a particle of mass m and friction coefficient γ moving in a force field F. The motion is described by the Langevin equations

$$\dot{q} = v, \quad m\dot{v} = -\gamma v + F(q) + \sqrt{2D_v}\xi,$$
 (35)

where ξ is a standard Gaussian white noise with unit variance. Since the associated path weight is

$$P(\omega) \sim \rho_0(x(0), v(0)) e^{\frac{\gamma}{2}t} \exp\left\{-\int_0^t dt' \frac{[m\dot{v}(t') + \gamma v(t') - F(t')]^2}{4D_v}\right\},$$
(36)

the time-integrated contraction rate of the noiseless dynamics, $Y(\omega) = \gamma t$, is singled out by comparison with an auxiliary dynamics having negative friction coefficient, i.e. $\gamma^* = -\gamma$. Recalling that time reversal here implies $\theta v(t') = -v(t-t')$, the analogous of (25) for underdamped diffusion is

$$\frac{P^*(\theta\omega)}{P(\omega)} = e^{\ln[\rho_t^*(x(t), -v(t))/\rho_0(x(0), v(0))] - \gamma t}.$$
 (37)

Essentially, this auxiliary dynamics emulates the time-reversal transformation of thermostated Hamiltonian systems. There [49], the friction coefficient γ is indeed replaced by the thermostat multiplier, that is an odd function of the velocity v and thus changes sign upon time inversion. Moreover, this auxiliary dynamics is equivalent to that used in Sec. III for underdamped diffusion, since $\gamma=1/\mu$ and we have already noticed that flipping the forces is the same as changing the sign of the mobility.

Similarly to the deterministic case, equations (25) and (37) can be turned into an integral FR for the dissipation function Ω [22],

$$\int_0^t \mathrm{d}t' \Omega(\boldsymbol{x}(t')) \equiv \ln \rho_0(\boldsymbol{x}(0)) - \ln \rho_0(\boldsymbol{x}(t)) + \int_0^t \mathrm{d}t' \sigma(\boldsymbol{x}(t')),$$

exploiting the freedom in choosing the initial density of the backward auxiliary trajectory. Specifically, taking $\rho_t^* = \rho_0$ in (25) we obtain the nonequilibrium partition identity, i.e. the integral version of the FR [14]

$$\left\langle \exp\left(-\int_0^t \mathrm{d}t'\Omega(t')\right)\right\rangle = 1,$$
 (38)

valid in overdamped diffusing systems for arbitrary initial densities and nonconservative forces. The same relation is obtained for underdamped diffusion from (37), provided that ρ_0 is independent of the sign of v, as it is, e.g., at equilibrium.

Finally, it is worth noting that the quantity (29) can also be related to the (finite-time) Lyapunov exponents Λ_i of the system. The latter are defined by considering the growth rates of k-dimensional volumes supported by k linearly independent perturbations $\delta \boldsymbol{x}^{(i)}$, with $1 \leq k \leq N$ [50]:

$$\operatorname{Vol}_{k}(\{\delta \boldsymbol{x}^{(i)}(t)\}) \sim e^{\sum_{i=1}^{k} \Lambda_{i} t}.$$
 (39)

The time evolution of such a perturbation δx in the initial condition of (31) is

$$\delta \dot{x}_i = F_i(\boldsymbol{x} + \delta \boldsymbol{x}) - F_i(\boldsymbol{x}) \approx (\partial_{x_i} F_j) \delta x_j \equiv (\nabla F)_{ij} \delta x_j,$$
(40)

which has the solution

$$\delta x_i(t) = \exp\left(\int_0^t \nabla F(t') dt'\right)_{ij} \delta x_j(0).$$
 (41)

Therefore, using the formula relating the determinant to the trace, $det(\exp A) = \exp(TrA)$, the relative variation

of the N-volume is obtained as

$$\det\left(\frac{\delta x_i(t)}{\delta x_j(0)}\right) = \exp\left(\int_0^t \partial_{x_i} F_i(t') dt'\right)$$
$$= \exp\left(-\int_0^t \sigma(t') dt'\right), \qquad (42)$$

which gives the time-averaged contraction rate in terms of the negative sum of all Lyapunov exponents,

$$\frac{1}{t} \int_0^t \sigma(t') dt' = -\sum_{i=1}^N \Lambda_i.$$
 (43)

If (31) is stochastic, as in the overdamped diffusion considered in the previous section, the Lyapunov exponents identify the separation rate of nearby trajectories subjected to the same noise realization, and Eqs. (25) and (27) are statements about the statistics of their spectrum. Note that Eqs. (27) and (25) can be restricted to quantities measured on subspaces of the full phase space using auxiliary dynamics where only some components of the forces are changed in sign. In particular, when $F_i^* = -F_i$ if i = k and $F_i^* = F_i$ otherwise, we get for example (no Einstein summation)

$$\left\langle \exp\left[-\frac{1}{D} \int_0^t dt' F_k(t') \dot{x}_k(t') + \int_0^t dt' \partial_{x_k} F_k(t')\right] \right\rangle = 1.$$
(44)

Since a k-volume is obtained as the determinant of the $k \times k$ minor of $\delta x_i(t)/\delta x_j(0)$, Eq. (44) relates a single Lyapunov exponent Λ_k ,

$$e^{t\Lambda_k} = \operatorname{Vol}_k(t) - \operatorname{Vol}_{k-1}(t) = \exp\left(\int_0^t dt' \partial_{x_k} F_k(t')\right),$$
(45)

to the entropy produced in the k direction.

V. CONCLUSIONS

We have introduced the concept of inflow rate. The fluctuations of its time integral are characterized by two fluctuation relations, one involving also boundary terms (density of states) and one involving the entropy production. In the continuum limit bringing jump systems to overdamped diffusion, the inflow rate becomes (minus) the divergence of forces, i.e. the phase space contraction rate. This quantity in reversible deterministic dynamical systems is known to be odd under time reversal. However, in general the phase space contraction rate can have any or no parity. In particular, in our case it results even under time reversal, due to the fact that the overdamped Langevin dynamics is not time reversible. Note that time reversibility is a condition commonly invoked in the derivations of FRs, hence it is sufficient, but it is known to be unnecessary [51–53].

We hope that these findings will be useful in developing nonequilibrium statistical mechanics —e.g. in deriving symmetry properties of response coefficients far

from equilibrium, as much as standard FRs are employed around equilibrium to obtain the Onsager reciprocity relations [54]— for which by now it is clear that we need not only to have entropy flows under control, but also to better understand the statistics of activities that have an

even parity under time reversal.

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- D. J. Evans, E. G. D. Cohen, and G. P. Morriss, "Probability of second law violations in shearing steady states," Phys. Rev. Lett. 71, 2401–2404 (1993).
- [2] D. J. Evans and D. J. Searles, "Equilibrium microstates which generate second law violating steady states," Phys. Rev. E 50, 1645–1648 (1994).
- [3] G. Gallavotti and E. G. D. Cohen, "Dynamical ensembles in nonequilibrium statistical mechanics," Phys. Rev. Lett. 74, 2694–2697 (1995).
- [4] G. Gallavotti and E. G. D. Cohen, "Dynamical ensembles in stationary states,," J. Stat. Phys. **80**, 931–970 (1995).
- [5] C. Jarzynski, "Nonequilibrium equality for free energy differences," Phys. Rev. Lett. 78, 2690 (1997).
- [6] C. Jarzynski, "Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach," Phys. Rev. E 56, 5018 (1997).
- [7] G. E. Crooks, "Nonequilibrium measurements of free energy differences for microscopically reversible Markovian systems," J. Stat. Phys. 90, 1481 (1998).
- [8] G. E. Crooks, "Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences," Phys. Rev. E 60, 2721 (1999) (1999).
- [9] J. Kurchan, "Fluctuation theorem for stochastic dynamics," J. Phys. A: Math. Gen 31, 3719-3729 (1998).
- [10] C. Maes, "The fluctuation theorem as a Gibbs property," J. Stat. Phys. 95, 367–392 (1999).
- [11] J. L. Lebowitz and H. Spohn, "A Gallavotti-Cohen-type symmetry in the large deviation functional for stochastic dynamics," J. Stat. Phys. 95, 333–365 (1999).
- [12] C. Maes, "On the origin and the use of fluctuation relations for the entropy," Séminaire Poincaré 2, 29–62 (2003).
- [13] U. Seifert, "Entropy production along a stochastic trajectory and an integral fluctuation theorem," Phys. Rev. Lett. 95, 040602 (2005).
- [14] D. J. Evans., D. J. Searles, and S. R. Williams, "On the fluctuation theorem for the dissipation function and its connection with response theory," J. Chem. Phys. 128, 014504 (2008).
- [15] V. Y. Chernyak, M Chertkov, and C. Jarzynski, "Pathintegral analysis of fluctuation theorems for general langevin processes," J. Stat. Mech., P08001 (2006).
- [16] R. J. Harris and G. M. Schütz, "Fluctuation theorems for stochastic dynamics," J. Stat. Mech., P07020 (2007).
- [17] M. Esposito, U. Harbola, and S. Mukamel, "Entropy fluctuation theorems in driven open systems: Application to electron counting statistics," Phys. Rev. E 76, 031132 (2007).
- [18] M. Esposito and C. Van den Broeck, "Three detailed fluctuation theorems," Phys. Rev. Lett. 104, 090601 (2010).

- [19] T. Sagawa and M. Ueda, "Fluctuation theorem with information exchange: Role of correlations in stochastic thermodynamics," Phys. Rev. Lett. 109, 180602 (2012).
- [20] H. K. Lee, C. Kwon, and H. Park, "Fluctuation theorems and entropy production with odd-parity variables," Phys. Rev. Lett. 110, 050602 (2013).
- [21] S. Rahav and U. Harbola, "An integral fluctuation theorem for systems with unidirectional transitions," J. Stat. Mech., P10044 (2014).
- [22] D. J. Evans and D. J. Searles, "The fluctuation theorem," Advances in Physics 51, 1529–1585 (2002).
- [23] L. Rondoni and C. Mejia-Monasterio, "Fluctuations in nonequilibrium statistical mechanics: models, mathematical theory, physical mechanisms," Nonlinearity 20, R1 (2007).
- [24] U. Marini Bettolo Marconi, A. Puglisi, L. Rondoni, and A. Vulpiani, "Fluctuation-dissipation: response theory in statistical physics," Phys. Rep. 461, 111–195 (2008).
- [25] U. Seifert, "Stochastic thermodynamics, fluctuation theorems and molecular machines," Rep. Prog. Phys. 75, 126001 (2012).
- [26] V. Lecomte, C. Appert-Rolland, and F. van Wijland, "Chaotic properties of systems with Markov dynamics," Phys. Rev. Lett. 95, 010601 (2005).
- [27] M. Merolle, J. P. Garrahan, and D. Chandler, "Spacetime thermodynampics of the glass transition," Proc. Natl. Acad. Sci. 102, 10837–10840 (2005).
- [28] C. Maes and M. H. van Wieren, "Time-symmetric fluctuations in nonequilibrium systems," Phys. Rev. Lett. 96, 240601 (2006).
- [29] V. Lecomte, C. Appert-Rolland, and F. van Wijland, "Thermodynamic formalism for systems with Markov dynamics," J. Stat. Phys. 127, 51–106 (2007).
- [30] J. P. Garrahan, R. L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, and F. van Wijland, "Dynamical firstorder phase transition in kinetically constrained models of glasses," Phys. Rev. Lett. 98, 195702 (2007).
- [31] J. P. Garrahan, R. L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, and F. van Wijland, "First-order dynamical phase transition in models of glasses: an approach based on ensembles of histories," J. Phys. A: Math. Gen 42, 075007 (2009).
- [32] M. Gorissen, J. Hooyberghs, and C. Vanderzande, "Density-matrix renormalization-group study of current and activity fluctuations near nonequilibrium phase transitions," Phys. Rev. E 79, 020101 (2009).
- [33] C. Maes and A. Salazar, "Active fluctuation symmetries," New J. Phys. 16, 015019 (2014).
- [34] E. Lippiello, F. Corberi, and M. Zannetti, "Offequilibrium generalization of the fluctuation dissipation theorem for Ising spins and measurement of the linear

- response function," Phys. Rev. E 71, 036104 (2005).
- [35] M. Baiesi, C. Maes, and B. Wynants, "Fluctuations and response of nonequilibrium states," Phys. Rev. Lett. 103, 010602 (2009).
- [36] M. Baiesi, E. Boksenbojm, C. Maes, and B. Wynants, "Linear response of nonequilibrium states, II: inertial dynamics," J. Stat. Phys. 139, 492–505 (2010).
- [37] M. Baiesi and C. Maes, "An update on the nonequilibrium linear response," New J. Phys. 15, 013004 (2013).
- [38] G. Falasco and M. Baiesi, "Temperature response in nonequilibrium stochastic systems," arXiv:1509.03139 (2015).
- [39] C. Maes, K. Netočný, and B. Wynants, "On and beyond entropy production; the case of Markov jump processes," Markov Proc. Rel. Fields 14, 445–464 (2008).
- [40] E. Autieri, P. Faccioli, M. Sega, F. Pederiva, and H. Orland, "Dominant reaction pathways in high-dimensional systems," J. Chem. Phys. 130, 064106 (2009).
- [41] E. Pitard, V. Lecomte, and F. van Wijland, "Dynamic transition in an atomic glass former: A molecular-dynamics evidence," Europhys. Lett. 96, 56002 (2011).
- [42] C. J. Fullerton and R. L. Jack, "Dynamical phase transitions in supercooled liquids: Interpreting measurements of dynamical activity," J. Chem. Phys. 138, 224506 (2013).
- [43] S. Katz, J. L. Lebowitz, and H. Spohn, "Phase transitions in stationary nonequilibrium states of model lattice systems," Phys. Rev. B 28, 1655–1658 (1983).
- [44] K. Mallick, "The exclusion process: A paradigm for non-equilibrium behaviour," Physica A 418, 17–48 (2015).
- [45] H. Risken, *The Fokker-Planck Equation*, 2nd ed. (Springer-Verlag, Berlin, 1989).

- [46] N. G. Van Kampen, Stochastic Processes in Physics and Chemistry, North-Holland Personal Library (Elsevier Science, 2011).
- [47] P. Castiglione, M. Falcioni, A. Lesne, and A. Vulpiani, Chaos and coarse graining in statistical mechanics (Cambridge University Press, London, 2008).
- [48] P. Gaspard, "Cycles, randomness, and transport from chaotic dynamics to stochastic processes," Chaos: An Interdisciplinary Journal of Nonlinear Science 25, 097606 (2015).
- [49] D. J. Evans and G. P. Morriss, Statistical Mechanics of NonEquilibrium Liquids, Theoretical Chemistry Monograph Series (Academic Press, London, 1990).
- [50] J. P. Eckmann and D. Ruelle, "Ergodic theory of chaos and strange attractors," Rev. Mod. Phys. 57, 617–656 (1985).
- [51] M. Colangeli, R. Klages, P. De Gregorio, and L. Rondoni, "Steady state fluctuation relations and time reversibility for non-smooth chaotic maps," J. Stat. Mech., P04021 (2011).
- [52] M. Colangeli and L. Rondoni, "Equilibrium, fluctuation relations and transport for irreversible deterministic dynamics," Physica D 241, 681–691 (2012).
- [53] M. Colangeli and L. Rondoni, "Fluctuation relations and nonequilibrium response for chaotic dissipative dynamics," in *Understanding Complex Systems - Applications* of Chaos and Nonlinear Dynamics in Science and Engineering, Vol. 3, edited by S. Banerjee and L. Rondoni (Springer Verlag Germany, Heidelberg, 2013) pp. 3–38.
- [54] G. Gallavotti, "Extension of Onsager's reciprocity to large fields and the chaotic hypothesis," Phys. Rev. Lett. 77, 4334–4337 (1996).