On correlations and fluctuations of time-averaged densities and currents with general time-dependence

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Abstract. We present technical results required for the description and understanding of correlations and fluctuations of the empirical density and current as well as diverse time-integrated and time-averaged thermodynamic currents of diffusion processes with a general time dependence on all time scales. In particular, we generalize the results from arXiv:2105.10483 (*Phys. Rev. Lett.*, article in press), arXiv:2204.06553 (*Phys. Rev. Research*, article in press), and arXiv:2206.04034 to additive functionals with explicit time dependence and transient or non-ergodic overdamped diffusion. As an illustration we apply the results to two-dimensional harmonically confined overdamped diffusion in a rotational flow evolving from a non-stationary initial distribution.

1. Introduction

"Time-average statistical mechanics" focuses on the study of additive functionals of stochastic paths and is important in the analysis of single-particle tracking [1–3], large deviation theory [4–8], and stochastic thermodynamics [9–16], to name but a few. The most important functionals from a physical point of view include the "empirical density" (also known as local or occupation time) [17–26], time-integrated and time-averaged currents [4–7, 15, 16, 27–35], and the time-averaged mean squared displacement (see e.g. [1,2,36-40]).

Fluctuations of time-averaged observables have a noise floor—they are bounded from below by the dissipation in a system, which is embodied within the "thermodynamic uncertainty relation" (TUR) [10, 41–49]. One may fruitfully exploit this universal lower bound on current fluctuations, e.g. to gauge the thermodynamic cost of precision [41,50,51], infer dissipation from fluctuations [34,35,43,44], or to derive thermodynamic limits on the temporal extent of anomalous diffusion [52].

Recent works addressed fluctuations of additive functionals in transient nonequilibrium systems [45–47], as well as in periodically [10, 48, 49] and generally driven systems [10]. Our aim here is to generalize the direct, stochastic-calculus approach we developed for steady-state systems in [34, 35] to transients and systems as well as functionals with explicit time dependence. Note that this includes non-ergodic systems (see e.g. [20, 25]).

The paper is structured as follows. We first set up the formal background and define the additive functionals in Sec. 2. In Section 3 we evaluate the first moments. In Sec. 4 we present our main result—a Lemma that allows a direct evaluation of fluctuations and correlations of general additive functionals in systems with explicit time dependence and derive general results for current fluctuations and current-density correlations. In Sec. 5 we illustrate how to apply the newly developed results by evaluating currentdensity correlations in overdamped diffusion in a rotational flow evolving from a nonstationary initial distribution. We conclude with a brief outlook.

2. Set-up

Consider overdamped Langevin dynamics with possibly multiplicative noise and explicit time dependence, described by the anti-Itô (or Hänggi-Klimontovich [53,54]) stochastic differential equation

$$d\mathbf{x}_{\tau} = \mathbf{F}(\mathbf{x}_{\tau}, \tau) d\tau + \boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \circledast d\mathbf{W}_{\tau}, \tag{1}$$

with positive definite diffusion matrix $\mathbf{D}(\mathbf{x}_{\tau}, \tau) = \boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau)\boldsymbol{\sigma}^{T}(\mathbf{x}_{\tau}, \tau)/2$. Assume that the drift $\mathbf{F}(\mathbf{x}_{\tau}, \tau)$ and noise amplitude $\boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau)$ are sufficiently well-behaved for Eq. (1) to be well-defined with a unique strong solution (e.g. assume that a weak solution exists and \mathbf{F} and $\boldsymbol{\sigma}$ are locally Lipschitz continuous [55]). The anti-Itô convention $\circledast d\mathbf{W}_{\tau} = \mathbf{W}_{\tau} - \mathbf{W}_{\tau-d\tau}$ is the thermodynamically consistent choice [13, 33, 35], in particular it ensures Boltzmann statistics if the drift $\mathbf{F}(\mathbf{x}_{\tau}, \tau)$ is such that the system settles into thermodynamic equilibrium [35]. The time-evolution of the probability density $P(\mathbf{x}, \tau)$ for any initial density $P(\mathbf{x}, \tau = 0)$ obeys a Fokker-Planck equation [56,57]

$$\partial_{\tau} P(\mathbf{x}, \tau) = \left[-\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{x}, \tau) + \nabla_{\mathbf{x}}^{T} \mathbf{D}(\mathbf{x}, \tau) \nabla_{\mathbf{x}} \right] P(\mathbf{x}, \tau)$$
$$\equiv L(\mathbf{x}, \tau) P(\mathbf{x}, \tau), \tag{2}$$

which is equivalent to a continuity equation $[\partial_{\tau} + \nabla_{\mathbf{x}} \cdot \hat{\mathbf{j}}(\mathbf{x}, \tau)]P(\mathbf{x}, \tau) = 0$, with the current operator

$$\hat{\mathbf{j}}(\mathbf{x},\tau) \equiv \mathbf{F}(\mathbf{x},\tau) - \mathbf{D}(\mathbf{x},\tau)\nabla_{\mathbf{x}}$$
 (3)

that gives the instantaneous current as $\mathbf{j}(\mathbf{x}, \tau) = \hat{\mathbf{j}}(\mathbf{x}, \tau)P(\mathbf{x}, \tau)$.

As a special case of Eq. (1) we will also study time-homogeneous non-equilibrium steady-state systems, where the stochastic equation of motion reads (curly brackets throughout denote that derivatives only act inside brackets)

$$d\mathbf{x}_{\tau} = \left[\mathbf{D}(\mathbf{x}_{\tau})\{\nabla \log p_{s}\}(\mathbf{x}_{\tau}) + \frac{\mathbf{j}_{s}(\mathbf{x}_{\tau})}{p_{s}(\mathbf{x}_{\tau})}\right] d\tau + \boldsymbol{\sigma}(\mathbf{x}_{\tau}) \circledast d\mathbf{W}_{\tau},$$
(4)

where $p_{\rm s}$ and $\mathbf{j}_{\rm s}$ denote the steady-state density and current [35]. Note that (as opposed to [34,35]) we do *not* assume that the initial distribution is sampled from $p_{\rm s}$.

Based on the dynamics defined in Eqs. (1) or (4), we consider time-averaged density and current functionals of the trajectories $[\mathbf{x}_{\tau}]_{0 \leq \tau \leq t}$ defined as

$$\rho_t^V = \frac{1}{t} \int_0^t V(\mathbf{x}_{\tau}, \tau) d\tau$$
$$\mathbf{J}_t^U = \frac{1}{t} \int_{\tau=0}^{\tau=t} U(\mathbf{x}_{\tau}, \tau) \circ d\mathbf{x}_{\tau},$$
(5)

with U, V differentiable and square integrable functions and \circ denotes the Stratonovich convention of the stochastic integral. The density functional ρ_t^V measures the time spent in the region $V(\mathbf{x}) \neq 0$, weighted by $V(\mathbf{x})$, while the current \mathbf{J}_t^U functional measures weighted displacements accumulated in U. In particular, for positive V, U that are centered around some point \mathbf{x} and decay on a finite length scale, one can interpret ρ_t^V and \mathbf{J}_t^U as the coarse-grained empirical density and current at \mathbf{x} [34, 35].

In the following, we will derive expressions for the mean values, correlations and fluctuations of these stochastic quantities and illustrate them with an example, thereby generalizing the results in [34,35] to non-steady-state initial conditions and even systems with explicit time-dependence, and thus in particular also without the existence of a steady state.

3. First moments

Consider overdamped Langevin dynamics as defined in Eq. (1) starting from an arbitrary initial density $P(\mathbf{x}, \tau = 0)$. Let $P(\mathbf{x}, \tau)$ be the probability density to find the particle at position \mathbf{x} after time τ , i.e. the solution of the Fokker-Planck equation in Eq. (2). Then the mean value of the density functional in Eq. (5) is given by

$$\left\langle \rho_t^V \right\rangle = \frac{1}{t} \int_0^t \left\langle V(\mathbf{x}_\tau, \tau) \right\rangle d\tau$$
$$= \frac{1}{t} \int_0^t d\tau \int d^d x V(\mathbf{x}, \tau) P(\mathbf{x}, \tau).$$
(6)

The mean value of the current is in turn given accordingly by (following closely the approach [35] using that the Itô-d \mathbf{W}_{τ} -term vanishes on average, integrating by parts,

$$\begin{split} \langle \mathbf{J}_{t}^{U} \rangle &= \frac{1}{t} \int_{0}^{t} \langle U(\mathbf{x}_{\tau}, \tau) \circ d\mathbf{x}_{\tau} \rangle \\ &= \frac{1}{t} \int_{\tau=0}^{\tau=t} \langle U(\mathbf{x}_{\tau}, \tau) d\mathbf{x}_{\tau} \rangle + \frac{1}{t} \int_{\tau=0}^{\tau=t} \frac{1}{2} \langle dU(\mathbf{x}_{\tau}, \tau) d\mathbf{x}_{\tau} \rangle_{s} \\ &= \frac{1}{t} \int_{0}^{t} d\tau \int d\mathbf{x} P(\mathbf{x}, \tau) \left[U(\mathbf{x}, \tau) \mathbf{F}(\mathbf{x}, \tau) + \left\{ \nabla_{\mathbf{x}}^{T} \mathbf{D}(\mathbf{x}, \tau) \right\} U(\mathbf{x}, \tau) + \mathbf{D}(\mathbf{x}, \tau) \left\{ \nabla_{\mathbf{x}} U(\mathbf{x}, \tau) \right\} \right] \\ &= \frac{1}{t} \int_{0}^{t} d\tau \int d\mathbf{x} P(\mathbf{x}, \tau) \left[U(\mathbf{x}, \tau) \mathbf{F}(\mathbf{x}, \tau) + \nabla_{\mathbf{x}}^{T} \mathbf{D}(\mathbf{x}, \tau) U(\mathbf{x}, \tau) \right] \\ &= \frac{1}{t} \int_{0}^{t} d\tau \int d\mathbf{x} U(\mathbf{x}, \tau) \left[\mathbf{F}(\mathbf{x}, \tau) - \mathbf{D}(\mathbf{x}, \tau) \nabla_{\mathbf{x}} \right] P(\mathbf{x}, \tau) \\ &= \frac{1}{t} \int_{0}^{t} d\tau \int d\mathbf{x} U(\mathbf{x}, \tau) \mathbf{j} \mathbf{j}(\mathbf{x}, \tau) P(\mathbf{x}, \tau) \\ &= \frac{1}{t} \int_{0}^{t} d\tau \int d\mathbf{x} U(\mathbf{x}, \tau) \mathbf{j} \mathbf{j}(\mathbf{x}, \tau) . \end{split}$$
(7)

The expressions Eq. (6) and (7) average the probability density and current over the function $U(\mathbf{x}, \tau)$ and over time $\tau \in [0, t]$, i.e. one can interpret ρ_t^V and \mathbf{J}_t^U as estimators of space and time averages of $P(\mathbf{x}, \tau)$ and $\mathbf{j}(\mathbf{x}, \tau)$. Note that for time-homogeneous steady-state dynamics (see Eq. (4)) these results are unchanged. They only further simplify for dynamics in Eq. (4) if also the initial condition is sampled from the steady state $P(\mathbf{x}, \tau = 0) = p_s(\mathbf{x})$, in which case $P(\mathbf{x}, \tau) = p_s(\mathbf{x})$ and $\mathbf{j}(\mathbf{x}, \tau) = \mathbf{j}_s(\mathbf{x})$ implies that $\langle \rho_t^V \rangle$ and $\langle \mathbf{J}_t^U \rangle$ become independent of t.

4. Correlations and fluctuations

and using $\mathbf{D} = \mathbf{D}^T$)

We now derive second moments and linear correlations of the time-averaged density and current in Eq. (5). The derivations for higher moments of currents are more involved than the first moments but as in [35] we solve the complications in the derivation by means of a single Lemma derived in the following subsection. Note that one could alternatively derive the following results using a Feynman-Kac approach (and optionally functional calculus) by appropriately generalizing the approach in [58].

4.1. Lemma

In the derivation of expressions for fluctuations and correlations of the time-averaged quantities we must evaluate correlations of noise increments $d\mathbf{W}_{\tau}$ and functions of $\mathbf{x}_{\tau'}$. Correlations for $\tau' \leq \tau$ vanish by the properties of the Wiener process. Conversely, correlations for $\tau' > \tau$ are non-trivial. This problem was solved for steady-state dynamics in [35] and via Doob conditioning [5, 13, 59] for general time-homogeneous Langevin systems in the Supplemental Material of [16]. We now generalize the direct approach from [35] to overdamped Langevin systems with explicit time-dependence.

Consider the k-th component $[\boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d} \mathbf{W}_{\tau}]_k$ of a noise increment in an expectation value $\langle f(\mathbf{x}_{\tau}, \mathbf{x}_{\tau'}, \tau, \tau') [\boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d} \mathbf{W}_{\tau}]_k \rangle$ with some (differentiable, square integrable) function f. For $\tau' \leq \tau$ this term vanishes due to vanishing correlations and zero mean of $\mathrm{d} \mathbf{W}_{\tau}$. Now consider $\tau' > \tau$.

Given a point $\mathbf{x}_{\tau} = \mathbf{x}$ and writing $\boldsymbol{\varepsilon} \equiv \boldsymbol{\sigma}(\mathbf{x}, \tau) d\mathbf{W}_{\tau}$, the equation of motion (1) rewritten in Itô form (writing out the anti-Itô correction term) implies a displacement $d\mathbf{x}_{\tau}(\mathbf{x}, \tau, \boldsymbol{\varepsilon}) = [\mathbf{F}(\mathbf{x}, \tau) + \nabla_{\mathbf{x}}^{T} \mathbf{D}(\mathbf{x}, \tau)] d\tau + \boldsymbol{\varepsilon}$. With this we can write the expectation $\langle f(\cdots) [\boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) d\mathbf{W}_{\tau}]_{k} \rangle$ as ε_{k} integrated over the probability to be at points $\mathbf{x}, \mathbf{x} + d\mathbf{x}_{\tau}(\mathbf{x}, \tau, \boldsymbol{\varepsilon}), \mathbf{y}$ at times $\tau < \tau + d\tau < \tau'$, i.e. (with joint density $P(\mathbf{y}, \tau'; \mathbf{x}, \tau)$ and conditional density $P(\mathbf{y}, \tau' | \mathbf{x}, \tau) \equiv P(\mathbf{y}, \tau'; \mathbf{x}, \tau)/P(\mathbf{x}, \tau)$; we write $\mathbb{1}_{\tau < \tau'}$ for 1 if $\tau < \tau'$ and 0 else)

where the probability $\mathbb{P}(\boldsymbol{\varepsilon})$ is given by a Gaussian distribution with zero mean and covariance matrix $2\mathbf{D}(\mathbf{x},\tau)d\tau$. Since this distribution is symmetric around **0**, only terms with even powers of the components of $\boldsymbol{\varepsilon}$ survive the $d\boldsymbol{\varepsilon}\mathbb{P}(\boldsymbol{\varepsilon})$ -integration. Note that

$$P(\mathbf{y},\tau'|\mathbf{x} + \mathrm{d}\mathbf{x}_{\tau}(\mathbf{x},\tau,\boldsymbol{\varepsilon}),\tau + \mathrm{d}\tau) \stackrel{\mathrm{d}\tau \to 0}{\longrightarrow} [1 + \mathrm{d}\mathbf{x}_{\tau}(\mathbf{x},\tau,\boldsymbol{\varepsilon}) \cdot \nabla_{\mathbf{x}}] P(\mathbf{y},\tau'|\mathbf{x},\tau) + \mathcal{O}(\mathrm{d}\tau), \quad (9)$$

and we can neglect the higher orders $\mathcal{O}(d\tau)$ since $\varepsilon_k \mathcal{O}(d\tau) = \mathcal{O}(d\tau^{3/2})$ which (unlike $\varepsilon_k \mathcal{O}(d\tau^{1/2})$) will still give zero after integration in τ . From the zeroth and first order contribution, we see that the only even power of the components of $\boldsymbol{\varepsilon}$ in the above integration gives

$$\langle f(\mathbf{x}_{\tau}, \mathbf{x}_{\tau'}, \tau, \tau') \left[\boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d} \mathbf{W}_{\tau} \right]_{k} \rangle$$

= $\mathbb{1}_{\tau < \tau'} \int \mathrm{d} \mathbf{x} \int \mathrm{d} \mathbf{y} f(\mathbf{x}, \mathbf{y}, \tau, \tau') P(\mathbf{x}, \tau) \int \mathrm{d} \boldsymbol{\varepsilon} \, \mathbb{P}(\boldsymbol{\varepsilon}) \varepsilon_{k} \boldsymbol{\varepsilon} \cdot \nabla_{\mathbf{x}} P(\mathbf{y}, \tau' | \mathbf{x}, \tau),$ (10)

which, using $\int d\boldsymbol{\varepsilon} \mathbb{P}(\boldsymbol{\varepsilon}) \varepsilon_k \varepsilon_j = 2D_{kj}(\mathbf{x}, \tau) d\tau$, yields the result for $\tau < \tau'$

$$\langle f(\mathbf{x}_{\tau}, \mathbf{x}_{\tau'}, \tau, \tau') \left[\boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d} \mathbf{W}_{\tau} \right]_{k} \rangle$$

= $\mathbb{1}_{\tau < \tau'} \mathrm{d} \tau \int \mathrm{d} \mathbf{x} \int \mathrm{d} \mathbf{y} P(\mathbf{x}, \tau) f(\mathbf{x}, \mathbf{y}, \tau, \tau') \left[2 \mathbf{D}(\mathbf{x}, \tau) \nabla_{\mathbf{x}} P(\mathbf{y}, \tau' | \mathbf{x}, \tau) \right]_{k}.$ (11)

For scalar products with vector valued functions **f** the result (11) can be summed over components f_k to obtain

$$\langle \mathbf{f}(\mathbf{x}_{\tau}, \mathbf{x}_{\tau'}, \tau, \tau') \cdot \boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d}\mathbf{W}_{\tau} \rangle$$

= $\mathbb{1}_{\tau < \tau'} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} P(\mathbf{x}, \tau) \mathbf{f}(\mathbf{x}, \mathbf{y}, \tau, \tau') \cdot 2 \mathbf{D}(\mathbf{x}, \tau) \nabla_{\mathbf{x}} P(\mathbf{y}, \tau' | \mathbf{x}, \tau).$ (12)

Eq. (12) is the central result of this work that allows us to directly deduce expressions for fluctuations and correlations of densities and currents. Upon integrating by parts and using symmetry $\mathbf{D}^T(\mathbf{x}, \tau) = \mathbf{D}(\mathbf{x}, \tau)$ Eq. (12) could also be rewritten as

$$\langle \mathbf{f}(\mathbf{x}_{\tau}, \mathbf{x}_{\tau'}, \tau, \tau') \cdot \boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d}\mathbf{W}_{\tau} \rangle$$

= $-\mathbb{1}_{\tau < \tau'} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} P(\mathbf{y}, \tau' | \mathbf{x}, \tau) \nabla_{\mathbf{x}} \cdot [P(\mathbf{x}, \tau) 2\mathbf{D}(\mathbf{x}, \tau) \mathbf{f}(\mathbf{x}, \mathbf{y}, \tau, \tau')].$ (13)

4.2. Fluctuations and correlations of densities and currents

Following the developed approach and generalizing the results obtained in [35] we now derive expressions for fluctuations and correlations of densities and currents for arbitrary initial conditions.

For two time-averaged densities ρ_t^U, ρ_t^V , the covariance (variance for U = V) is given by

$$\left\langle \rho_t^U \rho_t^V \right\rangle - \left\langle \rho_t^U \right\rangle \left\langle \rho_t^V \right\rangle = t^{-2} \int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \left[\left\langle U(\mathbf{x}_{\tau}, \tau) V(\mathbf{x}_{\tau'}, \tau') - \left\langle U(\mathbf{x}_{\tau}, \tau) \right\rangle \left\langle V(\mathbf{x}_{\tau'}, \tau') \right\rangle \right\rangle \right]$$
$$= t^{-2} \int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x}, \tau) V(\mathbf{y}, \tau') \left[P(\mathbf{x}, \tau; \mathbf{y}, \tau') - P(\mathbf{x}, \tau) P(\mathbf{y}, \tau') \right].$$
(14)

Note that this result can be interpreted as correlations caused by differences of $P(\mathbf{x}, \tau; \mathbf{y}, \tau')$ and $P(\mathbf{x}, \tau)P(\mathbf{y}, \tau')$, averaged over time and over functions U, V. More precisely, the two-point function $P(\mathbf{x}, \tau; \mathbf{y}, \tau')$ can be understood to be characterized by all paths with $\mathbf{x}_{\tau} = \mathbf{x}$ and $\mathbf{x}_{\tau'} = \mathbf{y}$. For further interpretation, in particular for the case of steady-state dynamics, see [34,35].

For the correlation of \mathbf{J}_t^U and ρ_t^V we first consider the expectation of the product and carry out the same steps as in Eq. (7),

$$t^{2} \left\langle \mathbf{J}_{t}^{U} \rho_{t}^{V} \right\rangle = \int_{0}^{t} \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_{\tau}, \tau) \circ \mathrm{d}\mathbf{x}_{\tau} V(\mathbf{x}_{\tau'}, \tau') \right\rangle$$
$$= \int_{0}^{t} \mathrm{d}\tau \int_{0}^{t} \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x}, \tau) V(\mathbf{y}, \tau') \hat{\mathbf{j}}(\mathbf{x}, \tau) P(\mathbf{y}, \tau'; \mathbf{x}, \tau)$$
$$+ \int_{0}^{t} \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_{\tau}, \tau) \boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d}\mathbf{W}_{\tau} V(\mathbf{x}_{\tau'}, \tau') \right\rangle.$$
(15)

Comparing with the calculation in Eq. (7), the noise term no longer vanishes since terms with $\tau < \tau'$ give non-trivial correlations according to Eq. (11), which in turn gives

$$\int_{0}^{t} \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_{\tau}, \tau) \boldsymbol{\sigma}(\mathbf{x}_{\tau}, \tau) \mathrm{d}\mathbf{W}_{\tau} V(\mathbf{x}_{\tau'}, \tau') \right\rangle = \int_{0}^{t} \mathrm{d}\tau' \int_{0}^{t} \mathrm{d}\tau \mathbb{1}_{\tau < \tau'} \times \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x}, \tau) V(\mathbf{y}, \tau') \left[2P(\mathbf{x}, \tau) \mathbf{D}(\mathbf{x}, \tau) \nabla_{\mathbf{x}} P(\mathbf{x}, \tau)^{-1} \right] P(\mathbf{y}, \tau'; \mathbf{x}, \tau),$$
(16)

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where we rewrote $P(\mathbf{y}, \tau' | \mathbf{x}, \tau) = P(\mathbf{x}, \tau)^{-1} P(\mathbf{y}, \tau'; \mathbf{x}, \tau)$. Introducing the adapted current operator

$$\hat{\mathbf{j}}^{\dagger}(\mathbf{x},\tau) \equiv \hat{\mathbf{j}}(\mathbf{x},\tau) + 2P(\mathbf{x},\tau)\mathbf{D}(\mathbf{x},\tau)\nabla_{\mathbf{x}}P(\mathbf{x},\tau)^{-1},$$
(17)

we thus obtain from Eq. (15) an expression for the current-density correlation that reads

$$\left\langle \mathbf{J}_{t}^{U} \rho_{t}^{V} \right\rangle - \left\langle \mathbf{J}_{t}^{U} \right\rangle \left\langle \rho_{t}^{V} \right\rangle = t^{-2} \int_{0}^{t} \mathrm{d}\tau \int_{0}^{t} \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x},\tau) V(\mathbf{y},\tau') \times \\ \left[\mathbbm{1}_{\tau > \tau'} \hat{\mathbf{j}}(\mathbf{x},\tau) + \mathbbm{1}_{\tau < \tau'} \hat{\mathbf{j}}^{\dagger}(\mathbf{x},\tau) \right] \left[P(\mathbf{y},\tau';\mathbf{x},\tau) - P(\mathbf{x},\tau) P(\mathbf{y},\tau') \right].$$
(18)

Note that to write the expression more compactly, we used that $\hat{\mathbf{j}}(\mathbf{x},\tau)P(\mathbf{x},\tau) = \hat{\mathbf{j}}^{\dagger}(\mathbf{x},\tau)P(\mathbf{x},\tau) = \mathbf{j}(\mathbf{x},\tau)$. For symmetry reasons and since the difference vanishes, we wrote $\mathbb{1}_{\tau > \tau'}$ instead of $\mathbb{1}_{\tau > \tau'}$.

The expression (18) is a natural generalization of Eq. (14) with the current operators $\hat{\mathbf{j}}, \hat{\mathbf{j}}^{\dagger}$ appearing. Recall that $\hat{\mathbf{j}}$ is the current operator entering the Fokker-Planck equation, see Eqs. (2)-(3). The adapted operator \hat{j}^{\dagger} defined in Eq. (17) accounts for the fact that trajectories contributing to $P(\mathbf{y}, \tau'; \mathbf{x}, \tau)$ that first visit \mathbf{x} and later \mathbf{y} (i.e. $\tau < \tau'$) have, compared to the Fokker-Planck evolution, altered statistics, since displacements at \mathbf{x} correlate with probabilities of reaching \mathbf{y} later. For the particular case of steady-state systems, the special case of the correlation result (18) and the adapted current operator were discussed in detail, and explained using a generalized time-reversal symmetry, in [34,35]. Note that for the case of time-homogeneous dynamics (in particular steadystate dynamics defined in Eq. (4)), the Fokker-Planck current operator Eq. (3) does not have an explicit time dependence such that $\hat{\mathbf{j}}(\mathbf{x},\tau)$ in Eq. (18) simplifies to $\hat{\mathbf{j}}(\mathbf{x})$. However, the adapted current operator $\hat{\mathbf{j}}^{\dagger}(\mathbf{x},\tau)$ defined in Eq. (17) retains explicit timedependence even for time-homogeneous dynamics. Only in the case of steady-state systems with steady-state initial conditions (where $P(\mathbf{x}, \tau) = p_{s}(\mathbf{x})$ for all τ) $\hat{\mathbf{j}}^{\dagger}$ has no explicit time dependence, and simplifies to the negative $\hat{\mathbf{j}}$ with inverted steady-state current $\mathbf{j}_{s} \rightarrow -\mathbf{j}_{s}$ [34,35].

Covariances of components m, n of time-integrated currents $J_{t,m}^U$ and $J_{t,n}^V$ can be obtained analogously by considering

$$t^{2} \left\langle J_{t,m}^{U} J_{t,n}^{V} \right\rangle = \int_{\tau'=0}^{\tau'=t} \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_{\tau}, \tau) \circ \mathrm{d} x_{\tau}^{m} V(\mathbf{x}_{\tau'}, \tau') \circ \mathrm{d} x_{\tau'}^{n} \right\rangle, \tag{19}$$

where both $\circ d\mathbf{x}_t$ increments split into dt and $d\mathbf{W}_t$ terms. The $d\tau d\tau'$ terms give rise to the current operator $\hat{\mathbf{j}}$ as in Eqs. (7),(15), but now its components $\hat{\mathbf{j}}_m(\mathbf{x},\tau)$ and $\hat{\mathbf{j}}_n(\mathbf{y},\tau')$ appear. The $dW_{\tau}dW_{\tau'}$ term yields (by Itô's isometry, i.e. "delta-correlated white noise")

$$\int_{\tau'=0}^{\tau'=t} \int_{\tau=0}^{\tau=t} \langle U(\mathbf{x}_{\tau},\tau) \left[\boldsymbol{\sigma}(\mathbf{x}_{\tau},\tau) \mathrm{d} \mathbf{W}_{\tau} \right]_{m} V(\mathbf{x}_{\tau'},\tau') \left[\boldsymbol{\sigma}(\mathbf{x}_{\tau'},\tau') \mathrm{d} \mathbf{W}_{\tau'} \right]_{n} \rangle$$
$$= \int_{0}^{t} \langle U(\mathbf{x}_{\tau},\tau) V(\mathbf{x}_{\tau},\tau) 2D_{mn}(\mathbf{x}_{\tau}) \rangle \mathrm{d}\tau$$
$$= 2 \int_{0}^{t} \mathrm{d}\tau \int \mathrm{d} \mathbf{x} U(\mathbf{x},\tau) V(\mathbf{x},\tau) D_{mn}(\mathbf{x}) P(\mathbf{x},\tau).$$
(20)

The mixed term $d\tau' d\mathbf{W}_{\tau}$ (and equivalently $d\tau d\mathbf{W}_{\tau'}$) in Eq. (19) according to calculations as in Eq. (7) and using Eq. (11) gives

$$\int_{0}^{t} \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \langle U(\mathbf{x}_{\tau},\tau) \left[\boldsymbol{\sigma}(\mathbf{x}_{\tau},\tau) \mathrm{d}\mathbf{W}_{\tau} \right]_{m} \left[V(\mathbf{x}_{\tau'},\tau') \mathbf{F}(\mathbf{x}_{\tau'},\tau') + \{\nabla \mathbf{D}V\}(\mathbf{x}_{\tau'},\tau') \right]_{n} \rangle = \mathbb{1}_{\tau < \tau'} \times \int_{0}^{t} \mathrm{d}\tau \int_{0}^{t} \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x},\tau) V(\mathbf{y},\tau') \hat{\mathbf{j}}_{n}(\mathbf{y},\tau') \left[2P(\mathbf{x},\tau) \nabla_{\mathbf{x}} P(\mathbf{x},\tau)^{-1} \right]_{m} P(\mathbf{y},\tau';\mathbf{x},\tau).$$

$$(21)$$

Collecting all terms and using the and notation \hat{j}_m^{\ddagger} for the components of \hat{j}^{\ddagger} in Eq. (17), we obtain for Eq. (19)

$$t^{2} \left\langle J_{t,m}^{U} J_{t,n}^{V} \right\rangle = 2 \int_{0}^{t} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} U(\mathbf{x},\tau) V(\mathbf{x},\tau) D_{mn}(\mathbf{x},\tau) P(\mathbf{x},\tau) + \int_{0}^{t} \mathrm{d}\tau \int_{0}^{t} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} \times U(\mathbf{x},\tau) V(\mathbf{y},\tau') \left[\mathbbm{1}_{\tau < \tau'} \hat{\mathbf{j}}_{m}^{\dagger}(\mathbf{x},\tau) \hat{\mathbf{j}}_{n}(\mathbf{y},\tau') + \mathbbm{1}_{\tau > \tau'} \hat{\mathbf{j}}_{m}(\mathbf{x},\tau) \hat{\mathbf{j}}_{n}^{\dagger}(\mathbf{y},\tau') \right] P(\mathbf{y},\tau';\mathbf{x},\tau).$$
(22)

From the derivation one sees that the first term is the $\tau = \tau'$ -contribution (see also [35]). This is the natural generalization of the results in Eqs. (14) and (18), with the interpretation of non-trivial displacements (and thus $\hat{\mathbf{j}}^{\dagger}$ instead of $\hat{\mathbf{j}}$) for currents evaluated at earlier times (see above and [34, 35]). As before, for time-homogeneous dynamics $\hat{\mathbf{j}}(\mathbf{x}, \tau)$ simplifies to $\hat{\mathbf{j}}(\mathbf{x})$ and in the special case of steady-state dynamics (see Eq. (4)) with steady-state initial conditions, $\hat{\mathbf{j}}^{\dagger}(\mathbf{x}, \tau)$ simplifies to $\hat{\mathbf{j}}^{\dagger}(\mathbf{x})$. This special case was discussed and explained using generalized time-reversal symmetry in [34, 35].

5. Example

To present a concrete minimal example, we consider a two-dimensional harmonically confined overdamped diffusion in a rotational flow (i.e. an irreversible Ornstein-Uhlenbeck process)

$$d\mathbf{x}_t = -\begin{bmatrix} 1 & -\Omega\\ \Omega & 1 \end{bmatrix} \mathbf{x} dt + \sqrt{2} d\mathbf{W}_t.$$
(23)

Assuming that the initial density $P(\mathbf{x}, \tau = 0)$ is Gaussian, the solution $P(\mathbf{x}, \tau)$ of the Fokker-Planck equation corresponding to Eq. (23) is well known to be a Gaussian density for all $\tau \ge 0$ (see e.g. [57]). We choose U to be a two-dimensional Gaussian centered at \mathbf{z} with width h, i.e.

$$U_{\mathbf{z}}(\mathbf{x}) = \frac{1}{2\pi h^2} \exp\left[-\frac{(\mathbf{x} - \mathbf{z})^2}{2h^2}\right].$$
 (24)

Due to the Gaussianity of $P(\mathbf{x}, \tau)$ and $U_{\mathbf{z}}(\mathbf{x})$, all spatial integrals entering the results Eqs. (14), (18) and (22) can be performed analytically, e.g. using the computer algebra system SymPy [60] (as outlined in the Supplemental Material of [34]). The two remaining time-integrals are computed numerically. For simplicity we only consider the (nonsteady-state) initial condition in a point, i.e. $P(\mathbf{x}, \tau = 0) = \delta(\mathbf{x} - \mathbf{x}_0)$. For this initial condition, via a left-right decomposition for the process Eq. (23) (see e.g. [56]) or by solving the Lyapunov equation, we have the time-dependent density

$$P(\mathbf{x},\tau) = \frac{1}{2\pi(1-e^{-2\tau})} \exp\left[\frac{-\left(\mathbf{x}-e^{-\tau}\begin{bmatrix}\cos(\Omega\tau) & \sin(\Omega\tau)\\-\sin(\Omega\tau) & \cos(\Omega\tau)\end{bmatrix}\mathbf{x}_0\right)^2}{2(1-e^{-2\tau})}\right],$$
(25)

i.e. the mean value $\langle \mathbf{x}_{\tau} \rangle = e^{-\tau} \begin{bmatrix} \cos(\Omega \tau) & \sin(\Omega \tau) \\ -\sin(\Omega \tau) & \cos(\Omega \tau) \end{bmatrix} \mathbf{x}_0$ moves on a spiral shape towards the center. The case $\Omega = 0$ corresponds to the equilibrium process, i.e. harmonically confined overdamped diffusion without rotational flow.

For this example, we compute the density-current correlation vector as in Eq. (18),

$$\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z},t;\mathbf{x}_{0}) \equiv \left\langle \mathbf{J}_{t}^{U_{\mathbf{z}}} \rho_{t}^{U_{\mathbf{z}}} \right\rangle_{\mathbf{x}_{0}} - \left\langle \mathbf{J}_{t}^{U_{\mathbf{z}}} \right\rangle_{\mathbf{x}_{0}} \left\langle \rho_{t}^{U_{\mathbf{z}}} \right\rangle_{\mathbf{x}_{0}} = t^{-2} \int_{0}^{t} \mathrm{d}\tau \int_{0}^{t} \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} \times U_{\mathbf{z}}(\mathbf{x}) U_{\mathbf{z}}(\mathbf{y}) \left[\mathbbm{1}_{\tau > \tau'} \hat{\mathbf{j}}(\mathbf{x}) + \mathbbm{1}_{\tau < \tau'} \hat{\mathbf{j}}^{\dagger}(\mathbf{x}, \tau) \right] \left[P(\mathbf{y}, \tau'; \mathbf{x}, \tau) - P(\mathbf{x}, \tau) P(\mathbf{y}, \tau') \right].$$
(26)

with Gaussian $U_{\mathbf{z}}$ as in Eq. (24). In Fig. 1 we show the time evolution and spatial dependence of this correlation vector. For long times without driving $\Omega = 0$, we see that $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0) \to 0$. This corresponds to the limit when the initial condition is forgotten, i.e. for long times $\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0)$ approaches the result of $\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t)$ for steady-state initial conditions where in equilibrium ($\Omega = 0$) we have $P(\mathbf{y}, \tau'; \mathbf{x}, \tau) = P(\mathbf{x}, \tau'; \mathbf{y}, \tau)$ (time-reversal symmetry) and $\mathbf{j}^{\dagger}(\mathbf{x}) = -\mathbf{j}(\mathbf{x})$ [35], implying $\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t) = \mathbf{0}$ at all \mathbf{z} . In the case $\Omega \neq 0$, the correlation $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0)$ becomes constant for long times, where $\mathbf{C}_{\mathbf{j}\rho} \propto t^{-1}$ represents the large-deviation limit of the correlation result, which agrees with the large-deviation limit for the process starting in steady-state initial conditions [35]. This has a spatial dependence similar to the steady-state current $\mathbf{j}_{\mathbf{s}}(\mathbf{z})$ but averaged over the Gaussian $U_{\mathbf{z}}$. By comparison with the color gradient we see in all panels in Fig. 1, as expected, that large values of the correlation can only occur at points that are visited for a significant amount of time, i.e. with not too small $\langle \rho_t^{U_{\mathbf{z}}} \rangle$.

In addition to the qualitative behavior shown in Fig. 1, we present a quantitative evaluation of the correlation result multiplied by time, $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0)$, for a single \mathbf{z} in Fig. 2. Simulations shown in Fig. 2 confirm the theoretical result in Eq. (18) (re-stated in Eq. (26)). As mentioned above this result approaches the large-deviation limit for long times. Moreover, for long times the initial condition will become irrelevant, i.e. $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0)$ approaches the result for $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t)$ for steady-state initial conditions [35]. First note that, due to the time-integration, deviations for short times are only slowly 'forgotten' with order t^{-1} (instead of exponentially fast with some Poincaré time scale). Interestingly, we see in Fig. 2a that for substantial coarse-graining (i.e. rather large



Figure 1. White arrows depict the correlation result multiplied by time, $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0)$ as in Eq. (18) with $\mathbf{x}_0 = (1, 1)^T$ for the process in Eq. (23) with $\Omega = 0$ in (a-d), $\Omega = 5$ in (e-h), and $U_{\mathbf{z}}$ as in Eq. (24). The position $\mathbf{z} = (z_1, z_2)^T$ around which the correlation is evaluated varies along the respective axes. The color gradient depicts the mean time-averaged density $\langle \rho_t^{U_{\mathbf{z}}} \rangle$, i.e. the time spent around \mathbf{z} weighted by $U_{\mathbf{z}}$. Time increases from left (a,e) to right (d,h), t = 0.3, 0.7, 2, 5

h = 0.5 in U_z in Eq. (24)), the result for $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0)$ starting in a point only approaches the corresponding value for steady-state initial condition (green curve) in the large deviation regime (black line), but *not* before. Going to smaller coarse graining h = 0.15in Fig. 2b, we see that the process starting in the center $\mathbf{x}_0 = (0, 0)^T$ (blue line) features the arguably more intuitive behavior, by first approaching the steady-state (green line) and later the large deviation result (black line). However, for a different initial condition (see orange line) the steady state curve is again only approached in the large deviation limit. This highlights the long-lasting and non-trivial effects of the time-integration and underscores why interpreting time-average observables, in particular those involving currents, remains challenging.

6. Conclusion

To summarize, we presented a new Lemma (12) that enabled us to derive results Eqs. (14), (18) and (22) for correlations and fluctuations of the time-averaged density and current Eq. (5) for general Langevin dynamics defined in Eq. (1) with general initial conditions. This generalization of the recent results derived for non-equilibrium steady states [34,35] may improve the understanding of inference of densities and currents with the estimators ρ_t^V and \mathbf{J}_t^U (in particular in connection with the notion of coarse graining [34,35]) in cases where the dynamics does *not* evolve from the steady-state, or is not



Figure 2. Quantitative depiction of the time-dependence of the x-component of the current-density correlation $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z},t;\mathbf{x}_0)_x$ with $\mathbf{z} = (0,-0.2)^T$ for the process in Eq. (23) with $\Omega = 3$ and $U_{\mathbf{z}}$ as in Eq. (24) with (a) h = 0.5 and (b) h = 0.15 for different initial conditions (colors). The new analytical result (blue and orange lines; Eq. (18)) is confirmed by simulations (crosses; for each t, (a) 10^5 and (b) 10^6 trajectories with 10^3 time-steps each were simulated according to the stochastic Euler algorithm). For $t \to \infty$, irrespective of the initial condition, all result approach the same large-deviation limit.

time-homogeneous. Importantly, the strategy of inferring dissipation from the current variance (see Eq. (22)) via the thermodynamic uncertainty relation (TUR) [41–44] remains valid. Generalized versions of the TUR, e.g. for general initial conditions [45] or time-dependent dynamics [10], already exist. A recently improved version of the TUR that includes current-density correlations (see Eq. (18)) is, however, so far only available for steady-state systems with steady-state initial conditions [15]. Notably, as we will show in a forthcoming publication, Lemma (12) allows the correlation-TUR to also be proved for transient dynamics.

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References

- A. Rebenshtok and E. Barkai, "Weakly non-ergodic statistical physics," J. Stat. Phys. 133 (2008) 565.
- [2] S. Burov, J.-H. Jeon, R. Metzler, and E. Barkai, "Single particle tracking in systems showing anomalous diffusion: the role of weak ergodicity breaking," *Phys. Chem. Chem. Phys.* 13 (2011) 1800.
- [3] R. Metzler, J.-H. Jeon, A. G. Cherstvy, and E. Barkai, "Anomalous diffusion models and their properties: non-stationarity, non-ergodicity, and ageing at the centenary of single particle tracking," *Phys. Chem. Chem. Phys.* 16 (2014) 24128.
- [4] H. Touchette, "The large deviation approach to statistical mechanics," Phys. Rep. 478 (2009) 1.
- [5] R. Chetrite and H. Touchette, "Nonequilibrium Markov processes conditioned on large deviations," *Annales Henri Poincaré* 16 (2014) 2005.
- [6] H. Touchette, "Introduction to dynamical large deviations of Markov processes," *Phys. A* 504 (2018) 5.

- [7] E. Mallmin, J. du Buisson, and H. Touchette, "Large deviations of currents in diffusions with reflective boundaries," J. Phys. A: Math. Theor. 54 (2021) 295001.
- [8] F. Coghi, R. Chetrite, and H. Touchette, "Role of current fluctuations in nonreversible samplers," *Phys. Rev. E* 103 (2021) 062142.
- [9] U. Seifert, "Stochastic thermodynamics: From principles to the cost of precision," *Phys. A* 504 (2018) 176.
- [10] T. Koyuk and U. Seifert, "Thermodynamic uncertainty relation for time-dependent driving," *Phys. Rev. Lett.* **125** (2020) 260604.
- [11] P. Pietzonka, A. C. Barato, and U. Seifert, "Universal bounds on current fluctuations," *Phys. Rev. E* 93 (2016) 052145.
- [12] U. Seifert, "Entropy production along a stochastic trajectory and an integral fluctuation theorem," *Phys. Rev. Lett.* **95** (2005) 040602.
- [13] S. Pigolotti, I. Neri, É. Roldán, and F. Jülicher, "Generic properties of stochastic entropy production," *Phys. Rev. Lett.* **119** (2017) 140604.
- [14] U. Seifert, "Stochastic thermodynamics, fluctuation theorems and molecular machines," *Rep.* Prog. Phys. 75 (2012) 126001.
- [15] A. Dechant and S.-i. Sasa, "Improving thermodynamic bounds using correlations," *Phys. Rev. X* 11 (2021) 041061.
- [16] A. Dechant and S.-i. Sasa, "Continuous time reversal and equality in the thermodynamic uncertainty relation," *Phys. Rev. Research* 3 (2021) 042012.
- [17] M. Kac, "On distributions of certain Wiener functionals," Trans. Am. Math. Soc. 65 (1949) 1.
- [18] D. A. Darling and M. Kac, "On occupation times for Markoff processes," Trans. Am. Math. Soc. 84 (1957) 444.
- [19] E. Aghion, D. A. Kessler, and E. Barkai, "From non-normalizable Boltzmann-Gibbs statistics to infinite-ergodic theory," *Phys. Rev. Lett.* **122** (2019) 010601.
- [20] S. Carmi and E. Barkai, "Fractional Feynman-Kac equation for weak ergodicity breaking," *Phys. Rev. E* 84 (2011) 061104.
- [21] S. N. Majumdar and A. Comtet, "Local and occupation time of a particle diffusing in a random medium," *Phys. Rev. Lett.* 89 (2002) 060601.
- [22] S. N. Majumdar and D. S. Dean, "Exact occupation time distribution in a non-Markovian sequence and its relation to spin glass models," *Phys. Rev. E* 66 (2002) 041102.
- [23] S. N. Majumdar, "Brownian functionals in physics and computer science," Curr. Sci. 89 (2005) 2075.
- [24] A. J. Bray, S. N. Majumdar, and G. Schehr, "Persistence and first-passage properties in nonequilibrium systems," Adv. Phys. 62 (2013) 225.
- [25] G. Bel and E. Barkai, "Weak ergodicity breaking in the continuous-time random walk," *Phys. Rev. Lett.* 94 (2005) 240602.
- [26] A. Lapolla, D. Hartich, and A. Godec, "Spectral theory of fluctuations in time-average statistical mechanics of reversible and driven systems," *Phys. Rev. Research* 2 (2020) 043084.
- [27] C. Maes, K. Netočný, and B. Wynants, "Steady state statistics of driven diffusions," Phys. A 387 (2008) 2675.
- [28] S. Kusuoka, K. Kuwada, and Y. Tamura, "Large deviation for stochastic line integrals as L^p -currents," *Probab. Theory Relat. Fields* 147 (2009) 649.
- [29] R. Chetrite and H. Touchette, "Nonequilibrium microcanonical and canonical ensembles and their equivalence," *Phys. Rev. Lett.* **111** (2013) 120601.
- [30] A. C. Barato and R. Chetrite, "A formal view on level 2.5 large deviations and fluctuation relations," J. Stat. Phys. 160 (2015) 1154.
- [31] J. Hoppenau, D. Nickelsen, and A. Engel, "Level 2 and level 2.5 large deviation functionals for systems with and without detailed balance," New J. Phys. 18 (2016) 083010.
- [32] C. Monthus, "Inference of Markov models from trajectories via large deviations at level 2.5 with applications to random walks in disordered media," J. Stat. Mech: Theory Exp. 2021 (2021)

063211.

- [33] D. Hartich and A. Godec, "Emergent memory and kinetic hysteresis in strongly driven networks," *Phys. Rev. X* 11 (2021) 041047.
- [34] C. Dieball and A. Godec, "Mathematical, thermodynamical, and experimental necessity for coarse graining empirical densities and currents in continuous space," arXiv:2105.10483 [cond-mat.stat-mech].
- [35] C. Dieball and A. Godec, "Coarse graining empirical densities and currents in continuous-space steady states," arXiv:2204.06553 [cond-mat.stat-mech].
- [36] D. S. Grebenkov, "Probability distribution of the time-averaged mean-square displacement of a gaussian process," *Phys. Rev. E* 84 (2011) 031124.
- [37] D. S. Grebenkov, "Time-averaged quadratic functionals of a gaussian process," *Phys. Rev. E* 83 (2011) 061117.
- [38] D. Boyer, D. S. Dean, C. Mejía-Monasterio, and G. Oshanin, "Optimal fits of diffusion constants from single-time data points of brownian trajectories," *Phys. Rev. E* 86 (2012) 060101.
- [39] D. Boyer, D. S. Dean, C. Mejía-Monasterio, and G. Oshanin, "Optimal estimates of the diffusion coefficient of a single brownian trajectory," *Phys. Rev. E* 85 (2012) 031136.
- [40] D. Boyer, D. S. Dean, C. Mejía-Monasterio, and G. Oshanin, "Distribution of the least-squares estimators of a single brownian trajectory diffusion coefficient," *Journal of Statistical Mechanics: Theory and Experiment* 2013 (2013) P04017.
- [41] A. C. Barato and U. Seifert, "Thermodynamic uncertainty relation for biomolecular processes," *Phys. Rev. Lett.* **114** (2015) 158101.
- [42] T. R. Gingrich, J. M. Horowitz, N. Perunov, and J. L. England, "Dissipation bounds all steady-state current fluctuations," *Phys. Rev. Lett.* **116** (2016) 120601.
- [43] T. R. Gingrich, G. M. Rotskoff, and J. M. Horowitz, "Inferring dissipation from current fluctuations," J. Phys. A: Math. Theor. 50 (2017) 184004.
- [44] J. M. Horowitz and T. R. Gingrich, "Thermodynamic uncertainty relations constrain non-equilibrium fluctuations," *Nat. Phys.* 16 (2019) 15–20.
- [45] A. Dechant and S.-i. Sasa, "Current fluctuations and transport efficiency for general Langevin systems," J. Stat. Mech: Theory Exp. 2018 (2018) 063209.
- [46] P. Pietzonka, F. Ritort, and U. Seifert, "Finite-time generalization of the thermodynamic uncertainty relation," *Phys. Rev. E* 96 (2017) 012101.
- [47] K. Liu, Z. Gong, and M. Ueda, "Thermodynamic uncertainty relation for arbitrary initial states," *Phys. Rev. Lett.* **125** (2020) 140602.
- [48] T. Koyuk and U. Seifert, "Operationally accessible bounds on fluctuations and entropy production in periodically driven systems," *Phys. Rev. Lett.* **122** (2019) 230601.
- [49] T. Koyuk, U. Seifert, and P. Pietzonka, "A generalization of the thermodynamic uncertainty relation to periodically driven systems," J. Phys. A 52 (2018) 02LT02.
- [50] A. C. Barato and U. Seifert, "Cost and precision of brownian clocks," *Phys. Rev. X* 6 (2016) 041053.
- [51] U. Seifert, "Stochastic thermodynamics: From principles to the cost of precision," *Physica A* 504 (2018) 176. Lecture Notes of the 14th International Summer School on Fundamental Problems in Statistical Physics.
- [52] D. Hartich and A. Godec, "Thermodynamic uncertainty relation bounds the extent of anomalous diffusion," *Phys. Rev. Lett.* **127** (2021) 080601.
- [53] P. Hänggi and H. Thomas, "Stochastic processes: Time evolution, symmetries and linear response," *Phys. Rep.* 88 (1982) 207–319.
- [54] Y. Klimontovich, "Ito, Stratonovich and kinetic forms of stochastic equations," *Physica A* 163 (1990) 515–532.
- [55] N. Ikeda and S. Watanabe, Stochastic Differential Equations and Diffusion Processes. North Holland, 1st edition ed., 1981. eBook ISBN: 9780080960128.
- [56] H. Risken, *The Fokker-Planck Equation*. Springer Berlin Heidelberg, 1989.

- [57] C. W. Gardiner, Handbook of stochastic methods for physics, chemistry, and the natural sciences. Springer-Verlag, Berlin New York, 1985.
- [58] C. Dieball and A. Godec, "Feynman-Kac theory of time-integrated functionals: Itô versus functional calculus," arXiv:2206.04034 [cond-mat.stat-mech].
- [59] J. L. Doob, "Conditional Brownian motion and the boundary limits of harmonic functions," Bull. Soc. Math. Fra. 85 (1957) 431.
- [60] A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, T. Rathnayake, S. Vig, B. E. Granger, R. P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson, F. Pedregosa, M. J. Curry, A. R. Terrel, v. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Scopatz, "SymPy: symbolic computing in Python," *PeerJ Comput. Sci.* 3 (2017) e103.