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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 Dieball and Godec (2022 *Phys. Rev. Lett.* **129** 140601); Dieball and Godec (2022 *Phys. Rev. Res.* **4** 033243); Dieball and Godec (2022 arXiv:2206.04034 [cond-mat.stat-mech]) 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.

Keywords: additive functionals of diffusion processes, overdamped Langevin dynamics, sample-to-sample fluctuations, time-average statistical mechanics, stochastic thermodynamics, stochastic calculus, Fokker–Planck equation

(Some figures may appear in colour only in the online journal)

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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 non-equilibrium 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 section 2. In section 3 we evaluate the first moments. In section 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 section 5 we illustrate how to apply the newly developed results by evaluating current-density correlations in overdamped diffusion in a rotational flow evolving from a non-stationary initial distribution. We conclude with a brief outlook.

2. Set-up

Consider overdamped Langevin dynamics (for details on deriving the overdamped limit see [53–55]) with possibly multiplicative noise and explicit time dependence, described by the anti-Itô (or Hänggi–Klimontovich [56, 57]) stochastic differential equation

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

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 equation (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 [58]). The anti-Itô convention $\circledast\mathrm{d}\mathbf{W}_\tau=\mathbf{W}_\tau-\mathbf{W}_{\tau-\mathrm{d}\tau}$ 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 [59, 60]

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

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

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

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 equation (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)

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

where p_s and $\mathbf{j}_\mathrm{s}$ 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_s.

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

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

with U, V differentiable and square integrable functions and $\circ$ denotes the Stratonovich convention of the stochastic integral. Reasons why the Stratonovich integral is the appropriate choice are detailed in [35]. 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 equation (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 equation (2). Then the mean value of the density functional in equation (5) is given by

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

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

$$
\begin{aligned}
\left\langle \mathbf{J}_t^U \right\rangle &= \frac{1}{t}\int_0^t \langle U(\mathbf{x}_\tau,\tau)\circ \mathrm{d}\mathbf{x}_\tau\rangle \\
&= \frac{1}{t}\int_{\tau=0}^{\tau=t} \langle U(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{x}_\tau\rangle + \frac{1}{t}\int_{\tau=0}^{\tau=t}\frac{1}{2}\langle \mathrm{d}U(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{x}_\tau\rangle_{\mathrm{s}} \\
&= \frac{1}{t}\int_0^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x} P(\mathbf{x},\tau)\left[U(\mathbf{x},\tau)\mathbf{F}(\mathbf{x},\tau) + \left\{\nabla_{\mathbf{x}}^T \mathbf{D}(\mathbf{x},\tau)\right\} U(\mathbf{x},\tau)\right. \\
&\quad \left. + \mathbf{D}(\mathbf{x},\tau)\left\{\nabla_{\mathbf{x}} U(\mathbf{x},\tau)\right\}\right] \\
&= \frac{1}{t}\int_0^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x} P(\mathbf{x},\tau)\left[U(\mathbf{x},\tau)\mathbf{F}(\mathbf{x},\tau) + \nabla_{\mathbf{x}}^T \mathbf{D}(\mathbf{x},\tau) U(\mathbf{x},\tau)\right] \\
&= \frac{1}{t}\int_0^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x} U(\mathbf{x},\tau)\left[\mathbf{F}(\mathbf{x},\tau) - \mathbf{D}(\mathbf{x},\tau)\nabla_{\mathbf{x}}\right] P(\mathbf{x},\tau) \\
&= \frac{1}{t}\int_0^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x} U(\mathbf{x},\tau)\hat{\mathbf{j}}(\mathbf{x},\tau) P(\mathbf{x},\tau) \\
&= \frac{1}{t}\int_0^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x} U(\mathbf{x},\tau)\mathbf{j}(\mathbf{x},\tau). \qquad (7)
\end{aligned}
$$

The expressions equations (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 equation (4)) these results are unchanged. They only further simplify for dynamics in equation (4) if also the initial condition is sampled from the steady state $P(\mathbf{x},\tau=0)=p_{\mathrm{s}}(\mathbf{x})$, in which case $P(\mathbf{x},\tau)=p_{\mathrm{s}}(\mathbf{x})$ and $\mathbf{j}(\mathbf{x},\tau)=\mathbf{j}_{\mathrm{s}}(\mathbf{x})$ implies that $\left\langle\rho_t^V\right\rangle$ and $\left\langle\mathbf{J}_t^U\right\rangle$ become independent of t.

4. Correlations and fluctuations

We now derive second moments and linear correlations of the time-averaged density and current in equation (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 [61].

4.1. Lemma

In the derivation of expressions for fluctuations and correlations of the time-averaged quantities we must evaluate correlations of noise increments $\mathrm{d}\mathbf{W}_\tau$ and functions of $\mathbf{x}_{\tau'}$. Correlations for $\tau'\leqslant\tau$ 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, 62] for general time-homogeneous Langevin systems in the Supplemental Material of [16]. Beyond the overdamped motion considered here, similar results can also obtained from the separation of slow and fast motion in more general systems [55]. We now generalize the direct approach from [35] to overdamped Langevin systems with explicit time-dependence.

Consider the kth component $[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau]_k$ of a noise increment in an expectation value $\left\langle f(\mathbf{x}_\tau,\mathbf{x}_{\tau'},\tau,\tau')\,[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau]_k\right\rangle$ with some (differentiable, square integrable) function f. For

$\tau' \leqslant \tau$ 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 $\boldsymbol{\varepsilon} \equiv \boldsymbol{\sigma}(\mathbf{x},\tau)\mathrm{d}\mathbf{W}_\tau$, the equation of motion (1) rewritten in Itô form (writing out the anti-Itô correction term) implies a displacement $\mathrm{d}\mathbf{x}_\tau(\mathbf{x},\tau,\boldsymbol{\varepsilon}) = [\mathbf{F}(\mathbf{x},\tau) + \nabla_\mathbf{x}^T\mathbf{D}(\mathbf{x},\tau)]\mathrm{d}\tau + \boldsymbol{\varepsilon}$. With this we can write the expectation $\left\langle f(\cdots)\left[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right]_k\right\rangle$ as ε_k integrated over the probability to be at points $\mathbf{x}, \mathbf{x} + \mathrm{d}\mathbf{x}_\tau(\mathbf{x},\tau,\boldsymbol{\varepsilon}), \mathbf{y}$ at times $\tau < \tau + \mathrm{d}\tau < \tau'$, 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)

$$\begin{aligned}&\left\langle f(\mathbf{x}_\tau,\mathbf{x}_{\tau'},\tau,\tau')\left[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right]_k\right\rangle\\ &\quad = \mathbb{1}_{\tau<\tau'}\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}f(\mathbf{x},\mathbf{y},\tau,\tau')\int\mathrm{d}\boldsymbol{\varepsilon}\,\mathbb{P}(\boldsymbol{\varepsilon})\varepsilon_k P(\mathbf{y},\tau'|\mathbf{x}+\mathrm{d}\mathbf{x}_\tau(\mathbf{x},\tau,\boldsymbol{\varepsilon}),\tau+\mathrm{d}\tau)P(\mathbf{x},\tau),\end{aligned} \tag{8}$$

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

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

and we can neglect the higher orders $\mathcal{O}(\mathrm{d}\tau)$ since $\varepsilon_k\mathcal{O}(\mathrm{d}\tau) = \mathcal{O}(\mathrm{d}\tau^{3/2})$ which (unlike $\varepsilon_k\mathcal{O}(\mathrm{d}\tau^{1/2})$) 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

$$\begin{aligned}&\left\langle f(\mathbf{x}_\tau,\mathbf{x}_{\tau'},\tau,\tau')\left[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right]_k\right\rangle\\ &\quad = \mathbb{1}_{\tau<\tau'}\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}f(\mathbf{x},\mathbf{y},\tau,\tau')P(\mathbf{x},\tau)\int\mathrm{d}\boldsymbol{\varepsilon}\,\mathbb{P}(\boldsymbol{\varepsilon})\varepsilon_k\boldsymbol{\varepsilon}\cdot\nabla_\mathbf{x}P(\mathbf{y},\tau'|\mathbf{x},\tau),\end{aligned} \tag{10}$$

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

$$\begin{aligned}&\left\langle f(\mathbf{x}_\tau,\mathbf{x}_{\tau'},\tau,\tau')\left[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right]_k\right\rangle\\ &\quad = \mathbb{1}_{\tau<\tau'}\mathrm{d}\tau\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}P(\mathbf{x},\tau)f(\mathbf{x},\mathbf{y},\tau,\tau')\left[2\mathbf{D}(\mathbf{x},\tau)\nabla_\mathbf{x}P(\mathbf{y},\tau'|\mathbf{x},\tau)\right]_k.\end{aligned} \tag{11}$$

For scalar products with vector valued functions $\mathbf{f}$ the result (11) can be summed over components f_k to obtain

$$\begin{aligned}&\left\langle \mathbf{f}(\mathbf{x}_\tau,\mathbf{x}_{\tau'},\tau,\tau')\cdot\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right\rangle\\ &\quad = \mathbb{1}_{\tau<\tau'}\mathrm{d}\tau\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}P(\mathbf{x},\tau)\mathbf{f}(\mathbf{x},\mathbf{y},\tau,\tau')\cdot 2\mathbf{D}(\mathbf{x},\tau)\nabla_\mathbf{x}P(\mathbf{y},\tau'|\mathbf{x},\tau).\end{aligned} \tag{12}$$

Equation (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 $\mathbf{D}^T(\mathbf{x},\tau) = \mathbf{D}(\mathbf{x},\tau)$ equation (12) could also be rewritten as

$$\begin{aligned}&\left\langle \mathbf{f}(\mathbf{x}_\tau,\mathbf{x}_{\tau'},\tau,\tau')\cdot\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right\rangle\\ &\quad = -\mathbb{1}_{\tau<\tau'}\mathrm{d}\tau\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}P(\mathbf{y},\tau'|\mathbf{x},\tau)\nabla_\mathbf{x}\cdot[P(\mathbf{x},\tau)2\mathbf{D}(\mathbf{x},\tau)\mathbf{f}(\mathbf{x},\mathbf{y},\tau,\tau')].\end{aligned} \tag{13}$$

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

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

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 equation (7),

$$t^2 \left\langle \mathbf{J}_t^U \rho_t^V \right\rangle = \int_0^t \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_\tau, \tau) \circ \mathrm{d}\mathbf{x}_\tau V(\mathbf{x}_{\tau'}, \tau') \right\rangle$$
$$= \int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x}, \tau) V(\mathbf{y}, \tau') \hat{\mathbf{j}}(\mathbf{x}, \tau) P(\mathbf{y}, \tau'; \mathbf{x}, \tau)$$
$$+ \int_0^t \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_\tau, \tau) \boldsymbol{\sigma}(\mathbf{x}_\tau, \tau) \mathrm{d}\mathbf{W}_\tau V(\mathbf{x}_{\tau'}, \tau') \right\rangle. \tag{15}$$

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

$$\int_0^t \mathrm{d}\tau' \int_{\tau=0}^{\tau=t} \left\langle U(\mathbf{x}_\tau, \tau) \boldsymbol{\sigma}(\mathbf{x}_\tau, \tau) \mathrm{d}\mathbf{W}_\tau V(\mathbf{x}_{\tau'}, \tau') \right\rangle$$
$$= \int_0^t \mathrm{d}\tau' \int_0^t \mathrm{d}\tau \mathbb{1}_{\tau < \tau'} \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x}, \tau) V(\mathbf{y}, \tau')$$
$$\times \left[2P(\mathbf{x}, \tau) \mathbf{D}(\mathbf{x}, \tau) \nabla_\mathbf{x} P(\mathbf{x}, \tau)^{-1} \right] P(\mathbf{y}, \tau'; \mathbf{x}, \tau), \tag{16}$$

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

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

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

$$\left\langle \mathbf{J}_t^U \rho_t^V \right\rangle - \left\langle \mathbf{J}_t^U \right\rangle \left\langle \rho_t^V \right\rangle = t^{-2} \int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} U(\mathbf{x}, \tau) V(\mathbf{y}, \tau')$$
$$\times \left[\mathbb{1}_{\tau > \tau'} \hat{\mathbf{j}}(\mathbf{x}, \tau) + \mathbb{1}_{\tau < \tau'} \hat{\mathbf{j}}^\ddagger(\mathbf{x}, \tau) \right] \left[P(\mathbf{y}, \tau'; \mathbf{x}, \tau) - P(\mathbf{x}, \tau) P(\mathbf{y}, \tau') \right]. \tag{18}$$

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

The expression (18) is a natural generalization of equation (14) with the current operators $\hat{\mathbf{j}}, \hat{\mathbf{j}}^\ddagger$ appearing. Recall that $\hat{\mathbf{j}}$ is the current operator entering the Fokker–Planck equation, see equations (2) and (3). The adapted operator $\hat{\mathbf{j}}^\ddagger$ defined in equation (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 steady-state dynamics defined in equation (4)), the Fokker–Planck current operator equation (3) does not have an explicit time dependence such that $\hat{\mathbf{j}}(\mathbf{x},\tau)$ in equation (18) simplifies to $\hat{\mathbf{j}}(\mathbf{x})$. However, the adapted current operator $\hat{\mathbf{j}}^{\ddagger}(\mathbf{x},\tau)$ defined in equation (17) retains explicit time-dependence even for time-homogeneous dynamics. Only in the case of steady-state systems with steady-state initial conditions (where $P(\mathbf{x},\tau)=p_{\mathrm{s}}(\mathbf{x})$ for all τ) $\hat{\mathbf{j}}^{\ddagger}$ has no explicit time dependence, and simplifies to the negative $\hat{\mathbf{j}}$ with inverted steady-state current $\mathbf{j}_{\mathrm{s}}\to-\mathbf{j}_{\mathrm{s}}$ [34, 35].

Covariances of components m,n of time-integrated currents $J^U_{t,m}$ and $J^V_{t,n}$ can be obtained analogously by considering

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

where both $\circ\mathrm{d}\mathbf{x}_t$ increments split into $\mathrm{d}t$ and $\mathrm{d}\mathbf{W}_t$ terms. The $\mathrm{d}\tau\mathrm{d}\tau'$ terms give rise to the current operator $\hat{\mathbf{j}}$ as in equations (7) and (15), but now its components $\hat{\mathrm{j}}_m(\mathbf{x},\tau)$ and $\hat{\mathrm{j}}_n(\mathbf{y},\tau')$ appear. The $\mathrm{d}W_\tau\mathrm{d}W_{\tau'}$ term yields (by Itô's isometry, i.e. 'delta-correlated white noise')

$$\begin{aligned}&\int_{\tau'=0}^{\tau'=t}\int_{\tau=0}^{\tau=t}\left\langle U(\mathbf{x}_\tau,\tau)\left[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right]_m V(\mathbf{x}_{\tau'},\tau')\left[\boldsymbol{\sigma}(\mathbf{x}_{\tau'},\tau')\mathrm{d}\mathbf{W}_{\tau'}\right]_n\right\rangle\\&\quad=\int_0^t\left\langle U(\mathbf{x}_\tau,\tau)V(\mathbf{x}_\tau,\tau)2D_{mn}(\mathbf{x}_\tau)\right\rangle\mathrm{d}\tau\\&\quad=2\int_0^t\mathrm{d}\tau\int\mathrm{d}\mathbf{x}U(\mathbf{x},\tau)V(\mathbf{x},\tau)D_{mn}(\mathbf{x})P(\mathbf{x},\tau).\end{aligned}\tag{20}$$

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

$$\begin{aligned}&\int_0^t\mathrm{d}\tau'\int_{\tau=0}^{\tau=t}\left\langle U(\mathbf{x}_\tau,\tau)\left[\boldsymbol{\sigma}(\mathbf{x}_\tau,\tau)\mathrm{d}\mathbf{W}_\tau\right]_m\left[V(\mathbf{x}_{\tau'},\tau')\mathbf{F}(\mathbf{x}_{\tau'},\tau')+\{\nabla\mathbf{D}V\}(\mathbf{x}_{\tau'},\tau')\right]_n\right\rangle\\&\quad=\mathbb{1}_{\tau<\tau'}\times\int_0^t\mathrm{d}\tau\int_0^t\mathrm{d}\tau'\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}U(\mathbf{x},\tau)V(\mathbf{y},\tau')\hat{\mathrm{j}}_n(\mathbf{y},\tau')\\&\qquad\times\left[2P(\mathbf{x},\tau)\nabla_{\mathbf{x}}P(\mathbf{x},\tau)^{-1}\right]_m P(\mathbf{y},\tau';\mathbf{x},\tau).\end{aligned}\tag{21}$$

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

$$\begin{aligned}t^2\left\langle J^U_{t,m}J^V_{t,n}\right\rangle&=2\int_0^t\mathrm{d}\tau\int\mathrm{d}\mathbf{x}\,U(\mathbf{x},\tau)V(\mathbf{x},\tau)D_{mn}(\mathbf{x},\tau)P(\mathbf{x},\tau)+\int_0^t\mathrm{d}\tau\int_0^t\mathrm{d}\tau'\int\mathrm{d}\mathbf{x}\int\mathrm{d}\mathbf{y}\\&\quad\times U(\mathbf{x},\tau)V(\mathbf{y},\tau')\left[\mathbb{1}_{\tau<\tau'}\hat{\mathrm{j}}^{\ddagger}_m(\mathbf{x},\tau)\hat{\mathrm{j}}_n(\mathbf{y},\tau')+\mathbb{1}_{\tau>\tau'}\hat{\mathrm{j}}_m(\mathbf{x},\tau)\hat{\mathrm{j}}^{\ddagger}_n(\mathbf{y},\tau')\right]P(\mathbf{y},\tau';\mathbf{x},\tau).\end{aligned}\tag{22}$$

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 equations (14) and (18), with the interpretation of non-trivial displacements (and thus $\hat{\mathbf{j}}^{\ddagger}$ 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 equation (4)) with steady-state initial conditions, $\hat{\mathbf{j}}^{\ddagger}(\mathbf{x},\tau)$ simplifies to $\hat{\mathbf{j}}^{\ddagger}(\mathbf{x})$. 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)

$$\mathrm{d}\mathbf{x}_t = -\begin{bmatrix} 1 & -\Omega \\ \Omega & 1 \end{bmatrix} \mathbf{x}\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{W}_t. \tag{23}$$

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 equation (23) is well known to be a Gaussian density for all $\tau \geqslant 0$ (see e.g. [60]). We choose U to be a two-dimensional Gaussian centered at $\mathbf{z}$ with width h, i.e.

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

Due to the Gaussianity of $P(\mathbf{x}, \tau)$ and $U_{\mathbf{z}}(\mathbf{x})$, all spatial integrals entering the results equations (14), (18) and (22) can be performed analytically, e.g. using the computer algebra system SymPy [63] (as outlined in the Supplemental Material of [34]). The two remaining time-integrals are computed numerically. For simplicity we only consider the (non-steady-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 equation (23) (see e.g. [59]) or by solving the Lyapunov equation, we have the time-dependent density

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

i.e. the mean value $\langle \mathbf{x}_\tau \rangle = \mathrm{e}^{-\tau}\begin{bmatrix} \cos(\Omega\tau) & \sin(\Omega\tau) \\ -\sin(\Omega\tau) & \cos(\Omega\tau) \end{bmatrix}\mathbf{x}_0$ 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 equation (18),

$$\begin{aligned} \mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t; \mathbf{x}_0) &\equiv \left\langle \mathbf{J}_t^{U_{\mathbf{z}}} \rho_t^{U_{\mathbf{z}}} \right\rangle_{\mathbf{x}_0} - \left\langle \mathbf{J}_t^{U_{\mathbf{z}}} \right\rangle_{\mathbf{x}_0} \left\langle \rho_t^{U_{\mathbf{z}}} \right\rangle_{\mathbf{x}_0} \\ &= t^{-2}\int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{y} \times U_{\mathbf{z}}(\mathbf{x}) U_{\mathbf{z}}(\mathbf{y}) \\ &\quad \times \left[\mathbb{1}_{\tau>\tau'}\hat{\mathbf{j}}(\mathbf{x}) + \mathbb{1}_{\tau<\tau'}\hat{\mathbf{j}}^{\ddagger}(\mathbf{x}, \tau)\right] \left[P(\mathbf{y}, \tau'; \mathbf{x}, \tau) - P(\mathbf{x}, \tau) P(\mathbf{y}, \tau')\right]. \end{aligned} \tag{26}$$

with Gaussian $U_{\mathbf{z}}$ as in equation (24). In figure 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 $\hat{\mathbf{j}}^{\ddagger}(\mathbf{x}) = -\hat{\mathbf{j}}(\mathbf{x})$ [35], implying $\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z}, t) = 0$ 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 $\mathbf{j}_{\mathrm{s}}(\mathbf{z})$ but averaged over the Gaussian $U_{\mathbf{z}}$. By comparison with the color gradient we see in all

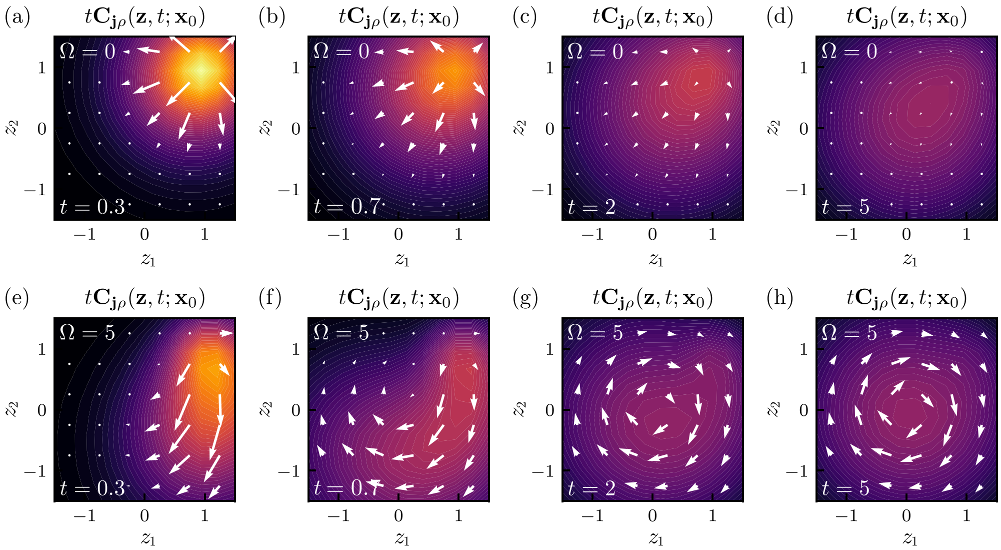

Figure 1. White arrows depict the correlation result multiplied by time, $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z},t;\mathbf{x}_0)$ as in equation (18) with $\mathbf{x}_0=(1,1)^T$ for the process in equation (23) with $\Omega=0$ in (a)–(d), $\Omega=5$ in (e)–(h), and $U_\mathbf{z}$ as in equation (24). 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), $t=0.3, 0.7, 2, 5$.

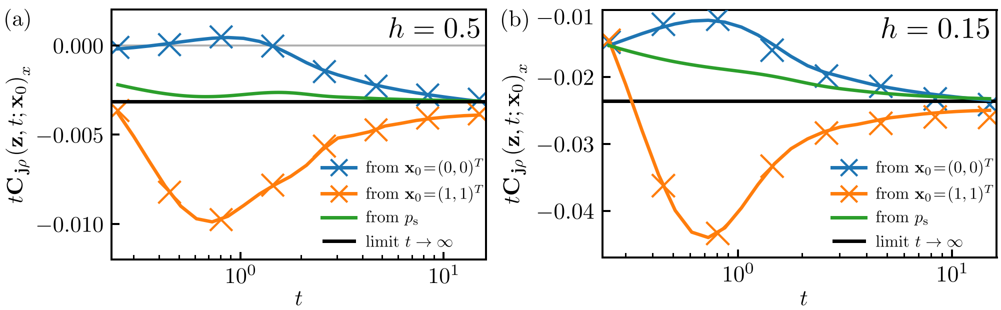

Figure 2. Quantitative depiction of the time-dependence of the x-component of the current-density correlation $t\mathbf{C}_{\mathbf{j}\rho}(\mathbf{z},t;\mathbf{x}_0)_x$ with $\mathbf{z}=(0,-0.2)^T$ for the process in equation (23) with $\Omega=3$ and $U_\mathbf{z}$ as in equation (24) with (a) $h=0.5$ and (b) $h=0.15$ for different initial conditions (colors). The new analytical result (blue and orange lines; equation (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.

panels in figure 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 figure 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 figure 2. Simulations shown in figure 2 confirm the theoretical result in equation (18) (re-stated in equation (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 figure 2(a) that for substantial coarse-graining (i.e. rather large $h=0.5$ in $U_{\mathbf{z}}$ in equation (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 $h=0.15$ in figure 2(b), 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 equations (14), (18) and (22) for correlations and fluctuations of the time-averaged density and current equation (5) for general Langevin dynamics defined in equation (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 time-homogeneous. Importantly, the strategy of inferring dissipation from the current variance (see equation (22)) via the 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 equation (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.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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