Feynman-Kac theory of time-integrated functionals: Itô versus functional calculus

Cai Dieball and Aljaž Godec

Mathematical bioPhysics Group, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

E-mail: agodec@mpinat.mpg.de

Abstract. The fluctuations of dynamical functionals such as the empirical density and current as well as heat, work and generalized currents in stochastic thermodynamics are often studied within the Feynman-Kac tilting formalism, which in the physics literature is typically derived by some form of Kramers-Moyal expansion. Here we derive the Feynman-Kac theory for general additive dynamical functionals directly via Itô calculus and via functional calculus, where the latter approach in fact appears to be new. Using Dyson series we then independently recapitulate recent results on steady-state (co)variances of general additive dynamical functionals derived in arXiv:2105.10483 and arXiv:2204.06553 directly from Itô calculus avoiding any tilting. We hope for our work to put the different approaches to stochastic functionals employed in the field on a common footing.

1. Introduction

Dynamical functionals such as local and occupation times, also known as the "empirical density", [1, 2, 3, 4, 5, 6, 7, 8, 9] as well as diverse time-integrated and time-averaged currents [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23] are central to "time-average statistical mechanics" [24, 25, 26], large deviation theory (see e.g. [11, 14, 17, 18, 27]), and path-wise, stochastic thermodynamics [28, 29, 30, 31, 32, 33, 20, 21]. Several techniques are available for the study of dynamical functionals, presumably best known is the Lie-Trotter-Kato formalism [2, 34] that was employed by Kac in his seminal work [1]. The techniques typically employed in physics rely on an analogy to quantum mechanical problems (see e.g. [7]) or assume some form of the Kramers-Moyal expansion [5, 35, 36, 8, 37, 38, 39] (see also interesting generalizations to anomalous dynamics [4, 9]).

In this technical paper we develop the Itô [40, 26] and functional calculus [41, 42] approaches to Feynman-Kac theory in the hope to better connect the often disjoint communities working on very similar problems. The outline of the paper is as follows. In Sec. 2.1 we provide the mathematical setup of the problem. In Sec. 2.2 we derive the Feynman-Kac equation for a general dynamical functional of diffusion processes using Itô calculus. By generalizing the approach by Fox [41, 42] we derive in Sec. 2.3 the

 $\mathbf{2}$

Feynman-Kac equation using functional calculus. In Sec. 3 we apply the formalism to compute steady-state (co)variances of general dynamical functionals using a Dyson-series approach. We conclude with a brief perspective.

2. Tilted Generator

2.1. Set-Up

We consider overdamped stochastic motion in d-dimensional space described by the stochastic differential equation

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

where $d\mathbf{W}_t$ is denotes increment of the Wiener process [40]. The corresponding diffusion constant is $\mathbf{D} = \boldsymbol{\sigma} \boldsymbol{\sigma}^T/2$. For simplicity we stick to additive noise whereas all present results generalize to multiplicative noise $\mathbf{D}(\mathbf{x})$ as described in [23]. In the physics literature Eq. (1) is typically written in the form of a Langevin equation

$$\dot{\mathbf{x}}_t = \mathbf{F}(\mathbf{x}_t) + \mathbf{f}(t),\tag{2}$$

with white noise amplitude $\langle \mathbf{f}(t)\mathbf{f}(t')^T \rangle = 2\mathbf{D}\delta(t-t')$. Comparing the two equations, $\mathbf{f}(t)$ corresponds to the derivative of \mathbf{W}_t , which however (with probability one) is not differentiable; more precisely, upon taking $dt \to 0$ one has $||d\mathbf{W}_t/dt|| = \infty$ with probability one, which is why the mathematics literature prefers Eq. (1).

If one describes the system on the level of probability densities instead of trajectories, the above equations translate to the Fokker-Planck equation $\partial_t G(\mathbf{x}, t | \mathbf{x}_0) = \hat{L}(\mathbf{x})G(\mathbf{x}, t | \mathbf{x}_0)$ with conditional density $G(\mathbf{x}, t | \mathbf{x}_0)$ to be at \mathbf{x} at time t after starting in \mathbf{x}_0 and the Fokker-Planck operator [43, 44]

$$\hat{L}(\mathbf{x}) = -\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{x}) + \nabla_{\mathbf{x}} \cdot \mathbf{D}\nabla_{\mathbf{x}} = -\nabla_{\mathbf{x}} \cdot \hat{\mathbf{j}}_{\mathbf{x}}, \qquad (3)$$

where we have defined the current operator $\hat{\mathbf{j}}_{\mathbf{x}} \equiv \mathbf{F}(\mathbf{x}) - \mathbf{D}\nabla_{\mathbf{x}}$. Although the approach presented here is more general, we restrict our attention to (possibly non-equilibrium) steady states where the drift $\mathbf{F}(\mathbf{x})$ is sufficiently smooth and confining to assure the existence of a steady-state (invariant) density $p_{\mathbf{s}}(\mathbf{x}) = \lim_{t\to\infty} G(\mathbf{x}, t | \mathbf{x}_0)$ and steadystate current $\mathbf{j}_{\mathbf{s}}(\mathbf{x}) = \hat{\mathbf{j}}_{\mathbf{x}} p_{\mathbf{s}}(\mathbf{x})$. The special case $\mathbf{j}_{\mathbf{s}}(\mathbf{x}) = \mathbf{0}$ corresponds to equilibrium steady states. For systems that eventually evolve into a steady state we can rewrite the current operator as [23]

$$\hat{\mathbf{j}}_{\mathbf{x}} = \mathbf{j}_{\mathrm{s}}(\mathbf{x})p_{\mathrm{s}}^{-1}(\mathbf{x}) - \mathbf{D}p_{\mathrm{s}}(\mathbf{x})\nabla_{\mathbf{x}}p_{\mathrm{s}}^{-1}(\mathbf{x}).$$
(4)

We will later also restrict the treatment to systems evolving from steady-state initial conditions, i.e. the initial condition $\mathbf{x}_{t=0}$ is drawn according to the density p_s .

We define the two fundamental additive dynamical functionals—time-integrated current and density—as

$$\mathbf{J}_{t} = \int_{\tau=0}^{\tau=t} U(\mathbf{x}_{\tau}) \circ \mathrm{d}\mathbf{x}_{\tau}$$
$$\rho_{t} = \int_{0}^{t} V(\mathbf{x}_{\tau}) \mathrm{d}\tau, \qquad (5)$$

with non-negative differentiable and square-integrable (real-valued) functions $U, V \colon \mathbb{R}^d \to \mathbb{R}$ and \circ denoting the Stratonovich integral. These objects depend on the whole trajectory $[\mathbf{x}_{\tau}]_{0 \leq \tau \leq t}$ and are thus random functionals with non-trivial statistics. In the following we will derive an equation for the characteristic function of the joint distribution of $\mathbf{x}_t, \rho_t, \mathbf{J}_t$ via a Feynman-Kac approach which will then yield the moments (including variances and correlations) via a Dyson series. The formalism was already applied to the time-averaged density ρ_t/t (under the term of local/occupation time fraction) [26, 45, 1]. To do so, we need to derive a tilted Fokker-Planck equation, which we first do via Itô calculus and then, equivalently, via a functional calculus. Note that the tilted generator can also be found in the literature on large deviation theory, see e.g. [15].

2.2. Tilting via Itô's Lemma

We first derive a tilted the Fokker-Planck equation using Itô calculus. From the Itô-Stratonovich correction term $dU(\mathbf{x}_{\tau})d\mathbf{x}_{\tau}/2$ and $d\mathbf{x}_{\tau}d\mathbf{x}_{\tau}^{T} = 2\mathbf{D}d\tau$ (where $\mathbf{D} = \boldsymbol{\sigma}\boldsymbol{\sigma}^{T}/2$) we obtain from Eqs. (1) and (5) the increments (curly brackets { $\nabla \dots$ } throughout denote that derivatives only act inside brackets)

$$d\mathbf{J}_{\tau} = U(\mathbf{x}_{\tau}) \circ d\mathbf{x}_{\tau} = U(\mathbf{x}_{\tau})d\mathbf{x}_{\tau} + \mathbf{D}\left\{\nabla U\right\}(\mathbf{x}_{\tau})d\tau$$
$$d\rho_{\tau} = V(\mathbf{x}_{\tau})d\tau.$$
(6)

We use Itô's Lemma [40] in d dimensions for a test function $f = f(\mathbf{x}_t, \rho_t, \mathbf{J}_t)$ and Eqs. (1) and (6), to obtain

$$df = \sum_{i=1}^{d} \frac{\partial f}{\partial x_{i}} dx_{t}^{i} + \frac{\partial f}{\partial \rho} d\rho_{t} + \sum_{i=1}^{d} \frac{\partial f}{\partial J_{i}} dJ_{t}^{i} + \frac{1}{2} \sum_{i,j=1}^{d} \left(\frac{\partial^{2} f}{\partial x_{i} \partial x_{j}} dx_{t}^{i} dx_{t}^{j} + \frac{\partial^{2} f}{\partial J_{i} \partial J_{j}} dJ_{t}^{i} dJ_{t}^{j} + 2 \frac{\partial^{2} f}{\partial x_{i} \partial J_{j}} dx_{t}^{i} dJ_{t}^{j} \right) = [(\nabla_{\mathbf{x}} f) + (\nabla_{\mathbf{J}} f) U(\mathbf{x}_{t})] [\mathbf{F}(\mathbf{x}_{t}) dt + \boldsymbol{\sigma} d\mathbf{W}_{t}] + (\nabla_{\mathbf{J}} f) \mathbf{D} \{\nabla_{\mathbf{x}} U\}(\mathbf{x}_{t}) dt + V(\mathbf{x}_{t}) \partial_{\rho} f dt + \left(\nabla_{\mathbf{x}}^{T} \mathbf{D} \nabla_{\mathbf{x}} + U(\mathbf{x}_{t})^{2} \nabla_{\mathbf{J}}^{T} \mathbf{D} \nabla_{\mathbf{J}} + 2U(\mathbf{x}_{t}) \nabla_{\mathbf{x}}^{T} \mathbf{D} \nabla_{\mathbf{J}} \right) f dt.$$
(7)

For the time derivative of f this gives

$$\frac{\mathrm{d}}{\mathrm{d}t}f(\mathbf{x}_{t},\rho_{t},\mathbf{J}_{t}) = \left[\left(\mathbf{F}+\boldsymbol{\sigma}\frac{\mathrm{d}\mathbf{W}_{t}}{\mathrm{d}t}\right)\left(\nabla_{\mathbf{x}}+U\nabla_{\mathbf{J}}\right)+\{\nabla_{\mathbf{x}}U\}\mathbf{D}\nabla_{\mathbf{J}}\right.\\\left.+V\partial_{\rho}+\nabla_{\mathbf{x}}^{T}\mathbf{D}\nabla_{\mathbf{x}}+U^{2}\nabla_{\mathbf{J}}^{T}\mathbf{D}\nabla_{\mathbf{J}}+2U\nabla_{\mathbf{x}}^{T}\mathbf{D}\nabla_{\mathbf{J}}\right]f(\mathbf{x}_{t},\rho_{t},\mathbf{J}_{t}).$$
(8)

Following this formalism, we move towards a tilted Fokker-Planck equation [1, 26]. Using the conditional probability density $Q_t(\mathbf{x}, \rho, \mathbf{J}|\mathbf{x}_0)$ we may write (omitting the \mathbf{x} dependence in \mathbf{F}, U, V for brevity) the evolution equation for $\langle f(\mathbf{x}_t, \rho_t, \mathbf{J}_t) \rangle_{\mathbf{x}_0}$, i.e. the expected value of $f(\mathbf{x}_t, \rho_t, \mathbf{J}_t)$ over the ensemble of paths propagating between \mathbf{x}_0 and \mathbf{x} in time t. Using Eq. (8) and integrating by parts, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle f(\mathbf{x}_{t},\rho_{t},\mathbf{J}_{t})\rangle_{\mathbf{x}_{0}} = \int \mathrm{d}^{d}x \int_{0}^{\infty} \mathrm{d}\rho \int \mathrm{d}^{d}J f(\mathbf{x},\rho,\mathbf{J})\partial_{t}Q_{t}(\mathbf{x},\rho,\mathbf{J}|\mathbf{x}_{0})$$

$$= \int \mathrm{d}^{d}x \int_{0}^{\infty} \mathrm{d}\rho \int \mathrm{d}^{d}J Q_{t}(\mathbf{x},\rho,\mathbf{J}|\mathbf{x}_{0})$$

$$\left[\mathbf{F}(\nabla_{\mathbf{x}}+U\nabla_{\mathbf{J}})+\{\nabla_{\mathbf{x}}U\}\mathbf{D}\nabla_{\mathbf{J}}+V\partial_{\rho}+\nabla_{\mathbf{x}}^{T}\mathbf{D}\nabla_{\mathbf{x}}+U^{2}\nabla_{\mathbf{J}}^{T}\mathbf{D}\nabla_{\mathbf{J}}+2U\nabla_{\mathbf{x}}^{T}\mathbf{D}\nabla_{\mathbf{J}}\right] f(\mathbf{x},\rho,\mathbf{J})$$

$$= \int \mathrm{d}^{d}x \int_{0}^{\infty} \mathrm{d}\rho \int \mathrm{d}^{d}J f(\mathbf{x},\rho,\mathbf{J}) \left[-\nabla_{\mathbf{x}}\mathbf{F}-U\mathbf{F}\nabla_{\mathbf{J}}-\{\nabla_{\mathbf{x}}U\}\mathbf{D}\nabla_{\mathbf{J}}-V\partial_{\rho} +\nabla_{\mathbf{x}}^{T}\mathbf{D}\nabla_{\mathbf{x}}+U^{2}\nabla_{\mathbf{J}}^{T}\mathbf{D}\nabla_{\mathbf{J}}+2U\nabla_{\mathbf{x}}^{T}\mathbf{D}\nabla_{\mathbf{J}}\right] Q_{t}(\mathbf{x},\rho,\mathbf{J}|\mathbf{x}_{0}).$$
(9)

Since the test function f is an arbitrary twice differentiable function, the resulting tilted Fokker-Planck equation reads

$$\partial_t Q_t(\mathbf{x}, \rho, \mathbf{J} | \mathbf{x}_0) = \hat{\mathcal{L}}_{\mathbf{x}, \rho, \mathbf{J}} Q_t(\mathbf{x}, \rho, \mathbf{J} | \mathbf{x}_0), \tag{10}$$

with the tilted Fokker-Planck operator (for discussion of the term $V\delta(\rho)$ entering at $\rho = 0$ see [26])

$$\hat{\mathcal{L}}_{\mathbf{x},\rho,\mathbf{J}} = -\nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{x}) + \nabla_{\mathbf{x}}^{T} \mathbf{D} \nabla_{\mathbf{x}} - V(\mathbf{x}) \partial_{\rho} - V(\mathbf{x}) \delta(\rho) - U(\mathbf{x}) \mathbf{F}(\mathbf{x}) \cdot \nabla_{\mathbf{J}} - \{\nabla_{\mathbf{x}} U(\mathbf{x})\}^{T} \mathbf{D} \nabla_{\mathbf{J}} + U(\mathbf{x})^{2} \nabla_{\mathbf{J}}^{T} \mathbf{D} \nabla_{\mathbf{J}} + 2 \nabla_{\mathbf{J}}^{T} \mathbf{D} \nabla_{\mathbf{x}} U(\mathbf{x}) = - [\nabla_{\mathbf{x}} + U(\mathbf{x}) \nabla_{\mathbf{J}}] \mathbf{F}(\mathbf{x}) - V(\mathbf{x}) \partial_{\rho} - V(\mathbf{x}) \delta(\rho) + [\nabla_{\mathbf{x}} + U(\mathbf{x}) \nabla_{\mathbf{J}}]^{T} \mathbf{D} [\nabla_{\mathbf{x}} + U(\mathbf{x}) \nabla_{\mathbf{J}}].$$
(11)

We see that the ρ dependence enters in standard Feynman-Kac form [1, 26], whereas the **J** dependence enters less trivially and shifts the gradient operator $\nabla_{\mathbf{x}} \to \nabla_{\mathbf{x}} + U(\mathbf{x})\nabla_{\mathbf{J}}$.

2.3. Tilting via functional calculus

We now re-derive the tilted Fokker-Planck operator in Eq. (11) using a functional calculus approach [41, 42] instead of the Itô calculus in the previous section. This shows that both alternative approaches are equivalent, as expected. Note that there is no need to work in discretized time (as opposed to [46]). We closely follow the derivation of the Fokker-Planck equation in Ref. [41] but for *d*-dimensional space and we generalize the approach to include the functionals defined in Eq. (5). The white noise term $\mathbf{f}(\tau)$ with $\langle \mathbf{f}(\tau)\mathbf{f}(\tau')^T \rangle_s = 2\mathbf{D}\delta(\tau - \tau')$ in the Langevin equation (2) can be considered to be described by a path-probability measure [41]

$$P[\mathbf{f}] = N \exp\left[-\frac{1}{2} \int_0^t \mathbf{f}(\tau) \mathbf{D}^{-1} \mathbf{f}(\tau) \mathrm{d}\tau\right], \qquad (12)$$

with normalization constant N which may be formally problematic but always cancels out.

We now derive a tilted Fokker-Planck equation for the joint conditional density Q of \mathbf{x}_t and the functionals \mathbf{J}_t, ρ_t , as defined in Eq. (5), given a deterministic initial condition \mathbf{x}_0 at time t = 0,

$$Q(\mathbf{x}, \rho, \mathbf{J}, t | \mathbf{x}_0) \equiv \int \mathcal{D} \mathbf{f} P[\mathbf{f}] \delta(\mathbf{x} - \mathbf{x}_t) \delta(\rho - \rho_t) \delta(\mathbf{J} - \mathbf{J}_t).$$
(13)

Note for the time derivatives that $\dot{\mathbf{J}}_t = U(\mathbf{x}_t)\dot{\mathbf{x}}_t$ and $\dot{\rho}_t = V(\mathbf{x}_t)$ to obtain (as a generalization of the calculation in Ref. [41] to dynamical functionals)

$$\partial_{t}Q(\mathbf{x},\rho,\mathbf{J},t|\mathbf{x}_{0}) = \partial_{t}\int \mathcal{D}\mathbf{f}P[\mathbf{f}]\delta(\mathbf{x}-\mathbf{x}_{t})\delta(\rho-\rho_{t})\delta(\mathbf{J}-\mathbf{J}_{t})$$

$$= \int \mathcal{D}\mathbf{f}P[\mathbf{f}] \left[-\nabla_{\mathbf{x}}\cdot\dot{\mathbf{x}}_{t} - \partial_{\rho}\dot{\rho}_{t} - \nabla_{\mathbf{J}}\cdot\dot{\mathbf{J}}_{t}\right]\delta(\mathbf{x}-\mathbf{x}_{t})\delta(\rho-\rho_{t})\delta(\mathbf{J}-\mathbf{J}_{t})$$

$$= \int \mathcal{D}\mathbf{f}P[\mathbf{f}] \left[-\nabla_{\mathbf{x}}\cdot[\mathbf{F}(\mathbf{x}_{t})+\mathbf{f}(t)] - V(\mathbf{x}_{t})\partial_{\rho} - U(\mathbf{x}_{t})\left[\mathbf{F}(\mathbf{x}_{t})+\mathbf{f}(t)\right]\nabla_{\mathbf{J}}\right]\times$$

$$\delta(\mathbf{x}-\mathbf{x}_{t})\delta(\rho-\rho_{t})\delta(\mathbf{J}-\mathbf{J}_{t})$$

$$= \left[-\nabla_{\mathbf{x}}\mathbf{F}(\mathbf{x}) - V(\mathbf{x})\partial_{\rho} - U(\mathbf{x})\mathbf{F}(\mathbf{x})\nabla_{\mathbf{J}}\right]Q(\mathbf{x},\rho,\mathbf{J},t|\mathbf{x}_{0})$$

$$- \left[\nabla_{\mathbf{x}}+U(\mathbf{x})\nabla_{\mathbf{J}}\right]\cdot\int \mathcal{D}\mathbf{f}P[\mathbf{f}]\mathbf{f}(t)\delta(\mathbf{x}-\mathbf{x}_{t})\delta(\rho-\rho_{t})\delta(\mathbf{J}-\mathbf{J}_{t}).$$
(14)

The functional derivative of Eq. (12) reads [41]

$$\frac{\delta P[\mathbf{f}]}{\delta \mathbf{f}(t)} = -\frac{1}{2} \mathbf{D}^{-1} \mathbf{f}(t) P[\mathbf{f}], \qquad (15)$$

which we use to obtain, via an integration by parts in $\delta \mathbf{f}(t)$,

$$-\int \mathcal{D}\mathbf{f} P[\mathbf{f}]\mathbf{f}(t)\delta(\mathbf{x} - \mathbf{x}_{t})\delta(\rho - \rho_{t})\delta(\mathbf{J} - \mathbf{J}_{t})$$

$$= 2\mathbf{D}\int \mathcal{D}\mathbf{f}\frac{\delta P[\mathbf{f}]}{\delta \mathbf{f}(t)}\delta(\mathbf{x} - \mathbf{x}_{t})\delta(\rho - \rho_{t})\delta(\mathbf{J} - \mathbf{J}_{t})$$

$$= -2\mathbf{D}\int \mathcal{D}\mathbf{f} P[\mathbf{f}]\frac{\delta}{\delta \mathbf{f}(t)}\delta(\mathbf{x} - \mathbf{x}_{t})\delta(\rho - \rho_{t})\delta(\mathbf{J} - \mathbf{J}_{t}).$$
(16)

Note that

$$\frac{\delta}{\delta \mathbf{f}(t)} \delta(\mathbf{x} - \mathbf{x}_t) \delta(\rho - \rho_t) \delta(\mathbf{J} - \mathbf{J}_t)$$
(17)

$$= \left[-\nabla_{\mathbf{x}} \frac{\delta \mathbf{x}_t}{\delta \mathbf{f}(t)} - \partial_{\rho} \frac{\delta \rho_t}{\delta \mathbf{f}(t)} - \nabla_{\mathbf{J}} \frac{\delta \mathbf{x}_t}{\delta \mathbf{f}(t)} \right] \delta(\mathbf{x} - \mathbf{x}_t) \delta(\rho - \rho_t) \delta(\mathbf{J} - \mathbf{J}_t),$$
(18)

and we use that $\delta \rho_t / \delta \mathbf{f}(t) = \mathbf{0}$, and $\delta \mathbf{x}_t / \delta \mathbf{f}(t) = \mathbf{1}/2$ [41] which implies $\delta \mathbf{J}_t / \delta \mathbf{f}(t) = U(\mathbf{x}_t)\mathbf{1}/2$, to get

$$\frac{\delta}{\delta \mathbf{f}(t)} \delta(\mathbf{x} - \mathbf{x}_t) \delta(\rho - \rho_t) \delta(\mathbf{J} - \mathbf{J}_t) = \frac{1}{2} \left[-\nabla_{\mathbf{x}} - U(\mathbf{x}_t) \nabla_{\mathbf{J}} \right] \delta(\mathbf{x} - \mathbf{x}_t) \delta(\rho - \rho_t) \delta(\mathbf{J} - \mathbf{J}_t).$$
(19)

Plugging Eq. (19) first into Eq. (16) and then into Eq. (14) yields the tilted Fokker-Planck equation for the joint conditional density (with the $-V(\mathbf{x})\delta(\rho)$ term entering as above and in [26])

$$\partial_{t}Q(\mathbf{x},\rho,\mathbf{J},t|\mathbf{x}_{0}) = \left[-\nabla_{\mathbf{x}}\mathbf{F}(\mathbf{x}) - V(\mathbf{x})\partial_{\rho} - V(\mathbf{x})\delta(\rho) - U(\mathbf{x})\mathbf{F}(\mathbf{x})\nabla_{\mathbf{J}} + \left[\nabla_{\mathbf{x}} + U(\mathbf{x})\nabla_{\mathbf{J}}\right]^{T}\mathbf{D}\left[\nabla_{\mathbf{x}} + U(\mathbf{x})\nabla_{\mathbf{J}}\right]\right]Q(\mathbf{x},\rho,\mathbf{J},t|\mathbf{x}_{0}).$$
(20)

Note that Eq. (20) fully agrees with Eq. (11) derived via Itô calculus thus establishing the announced equivalence of the two approaches.

3. Steady-state covariance via Dyson expansion of the tilted propagator

We now derive the moments of the dynamical functionals Eq. (5) from a Dyson expansion. First, let us consider a one-dimensional Laplace variable v and a *d*dimensional Fourier variable $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_d)$ and Laplace and Fourier transform $Q_t(\mathbf{x}, \rho, \mathbf{J} | \mathbf{x}_0)$ as

$$\tilde{Q}_t(\mathbf{x}, v, \boldsymbol{\omega} | \mathbf{x}_0) \equiv \int_0^\infty \mathrm{d}\rho \int \mathrm{d}^d J \, Q_t(\mathbf{x}, \rho, \mathbf{J} | \mathbf{x}_0) \exp\left(-v\rho - \mathrm{i}\boldsymbol{\omega} \cdot \mathbf{J}\right).$$
(21)

Recall the Fokker-Planck operator $\hat{L}(\mathbf{x}) = -\nabla_{\mathbf{x}} \cdot \hat{\mathbf{j}}_{\mathbf{x}}$ with the current operator $\hat{\mathbf{j}}_{\mathbf{x}} = \mathbf{F}(\mathbf{x}) - \mathbf{D}\nabla_{\mathbf{x}}$ from Eq. (3). The Fourier-Laplace transform of the tilted Fokker-Planck operator in Eqs. (11) and (20) reads

$$\hat{\mathcal{L}}(\mathbf{x}, v, \boldsymbol{\omega}) = \hat{L}(\mathbf{x}) - vV(\mathbf{x}) - i\boldsymbol{\omega}^T \cdot \hat{\mathbf{L}}^U(\mathbf{x}) - U(\mathbf{x})^2 \boldsymbol{\omega}^T \mathbf{D} \boldsymbol{\omega}$$
$$\hat{\mathbf{L}}^U(\mathbf{x}) \equiv U(\mathbf{x}) \hat{\mathbf{j}}_{\mathbf{x}} - \mathbf{D} \nabla_{\mathbf{x}} U(\mathbf{x}).$$
(22)

Note that compared to the tilt of the density (i.e. the *v*-term; see also [26]), the tilt corresponding to the current observable ($\boldsymbol{\omega}$ -terms) involves more terms and even a term that is second order in $\boldsymbol{\omega}$. The second order term occurs since $(\mathbf{dW}_{\tau})^2 \sim \mathbf{d\tau}$ and therefore (in contrast to $\mathbf{d\tau}\mathbf{dW}_{\tau}$ and $\mathbf{d\tau}^2$) contributes in the tilting of the generator.

We now restrict our attention to dynamics starting in the steady state p_s and denote the average over an ensemble over paths propagating from the steady state by $\langle \cdot \rangle_s$. Extensions of the formalism to any initial distribution are straightforward and introduce additional transient terms. The moment generating function (also known as characteristic function) reads

$$\tilde{\mathcal{P}}_{t}^{\rho\mathbf{J}}(v,\boldsymbol{\omega}|p_{s}) \equiv \left\langle \mathrm{e}^{-v\rho_{t}-\mathrm{i}\boldsymbol{\omega}\cdot\mathbf{J}_{t}} \right\rangle_{s} = 1 - v \left\langle \rho_{t} \right\rangle_{s} - \mathrm{i}\boldsymbol{\omega}\cdot\left\langle \mathbf{J}_{t} \right\rangle_{s} + \mathrm{i}v\boldsymbol{\omega}\cdot\left\langle \rho_{t}\mathbf{J}_{t} \right\rangle_{s} + O(\boldsymbol{\omega}^{2},v^{2}).$$
(23)

The Dyson expansion allows to expand the tilted generator as (also see [26])

$$e^{\hat{\mathcal{L}}(\mathbf{x}_{1},v,\boldsymbol{\omega})t} = 1 + \int_{0}^{t} dt_{1}e^{\hat{\mathcal{L}}(\mathbf{x}_{1})(t-t_{1})} \left[vV(\mathbf{x}_{1}) + i\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] e^{\hat{\mathcal{L}}(\mathbf{x}_{1})t_{1}} + \int_{0}^{t} dt_{2} \int_{0}^{t_{2}} dt_{1}e^{\hat{\mathcal{L}}(\mathbf{x}_{1})(t-t_{2})} \left[vV(\mathbf{x}_{1}) + i\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] e^{\hat{\mathcal{L}}(\mathbf{x}_{1})(t_{2}-t_{1})} \left[vV(\mathbf{x}_{1}) + i\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] e^{\hat{\mathcal{L}}(\mathbf{x}_{1})t_{1}} + O(\boldsymbol{\omega}^{2}, v^{2}).$$
(24)

Using that the first propagation only differs from 1 by total derivatives (recall $\hat{L}(\mathbf{x}) = -\nabla_{\mathbf{x}} \cdot \hat{\mathbf{j}}_{\mathbf{x}}$), and using for the last propagation term $e^{\hat{L}(\mathbf{x}_1)t_1} p_s(\mathbf{x}_1) = p_s(\mathbf{x}_1)$, we obtain

$$\tilde{\mathcal{P}}_{t}^{\rho \mathbf{J}}(v, \boldsymbol{\omega}|p_{s}) = \int \mathrm{d}^{d}x_{1} \,\mathrm{e}^{\hat{\mathcal{L}}(\mathbf{x}_{1}, v, \boldsymbol{\omega})t} p_{s}(\mathbf{x}_{1})$$

$$=1 + \int \mathrm{d}^{d}x_{1} \int_{0}^{t} \mathrm{d}t_{1} \left[vV(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] p_{s}(\mathbf{x}_{1})$$

$$+ \sum_{l,m=1}^{d} \int \mathrm{d}^{d}x_{1} \int_{0}^{t} \mathrm{d}t_{2} \int_{0}^{t_{2}} \mathrm{d}t_{1} \left[vV(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] \mathrm{e}^{\hat{\mathcal{L}}(\mathbf{x}_{1})(t_{2}-t_{1})}$$

$$\left[vV(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] p_{s}(\mathbf{x}_{1}) + O(\boldsymbol{\omega}^{2}, v^{2}).$$
(25)

We replace the one-step propagation by the conditional density $G(\mathbf{x}_2, t | \mathbf{x}_1) = e^{\hat{L}(\mathbf{x}_1)t} \delta(\mathbf{x}_2 - \mathbf{x}_1),$

$$\int \mathrm{d}^d x_1 f(\mathbf{x}_1) \mathrm{e}^{\hat{L}(\mathbf{x}_1)(t_2 - t_1)} g(\mathbf{x}_1) = \int \mathrm{d}^d x_1 \int \mathrm{d}^d x_2 f(\mathbf{x}_2) G(\mathbf{x}_2, t_2 - t_1 | \mathbf{x}_1) g(\mathbf{x}_1), \quad (26)$$

which yields

$$\tilde{\mathcal{P}}_{t}^{\rho \mathbf{J}}(v,\boldsymbol{\omega}|p_{s}) = 1 + \int \mathrm{d}^{d}x_{1} \int_{0}^{t} \mathrm{d}t_{1} \left[vV(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] p_{s}(\mathbf{x}_{1}) \\ + \int \mathrm{d}^{d}x_{1} \int \mathrm{d}^{d}x_{2} \int_{0}^{t} \mathrm{d}t_{2} \int_{0}^{t_{2}} \mathrm{d}t_{1} \left[vV(\mathbf{x}_{2}) + \mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{2}) \right] \\ G(\mathbf{x}_{2}, t_{2} - t_{1}|\mathbf{x}_{1}) \left[vV(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) \right] p_{s}(\mathbf{x}_{1}) + O(\boldsymbol{\omega}^{2}, v^{2}).$$
(27)

Comparing the definition and expansion of the characteristic function Eq. (23) with the result Eq. (27) from the Dyson expansion, we obtain the moments and correlations of the functionals $\mathbf{J}_t = \int_{\tau=0}^{\tau=t} U(\mathbf{x}_{\tau}) \circ \mathrm{d}\mathbf{x}_{\tau}$ and $\rho_t = \int_0^t V(\mathbf{x}_{\tau}) \mathrm{d}\tau$.

Note that the first moments (i.e. the mean values for steady-state initial conditions) can also be obtained directly [23, 10] but we obtain them here by comparing Eqs. (23) and Eq. (27),

$$\langle \rho_t \rangle_{\mathbf{s}} = \int_0^t \mathrm{d}t_1 \int \mathrm{d}^d x_1 V(\mathbf{x}_1) p_{\mathbf{s}}(\mathbf{x}_1) = t \int \mathrm{d}^d x_1 V(\mathbf{x}_1) p_{\mathbf{s}}(\mathbf{x}_1)$$

$$\langle \mathbf{J}_t \rangle_{\mathbf{s}} = t \int \mathrm{d}^d x_1 [U(\mathbf{x}_1) \hat{\mathbf{j}}_{\mathbf{x}_1} - \mathbf{D} \nabla_{\mathbf{x}_1} U(\mathbf{x}_1)] p_{\mathbf{s}}(\mathbf{x}_1) = t \int \mathrm{d}^d x_1 U(\mathbf{x}_1) \mathbf{j}_{\mathbf{s}}(\mathbf{x}_1), \quad (28)$$

where $\nabla_{\mathbf{x}_1} U(\mathbf{x}_1) p_{\mathbf{s}}(\mathbf{x}_1)$ vanishes after integration by parts and $\mathbf{j}_{\mathbf{s}}(\mathbf{x}_1) \equiv \hat{\mathbf{j}}_{\mathbf{x}_1} p_{\mathbf{s}}(\mathbf{x}_1)$ is the steady-state current.

By comparing once more Eqs. (23) and Eq. (27) we have for the steady-state

expectation $\langle \mathbf{J}_t \rho_t \rangle_s$ that

$$\langle \mathbf{J}_{t} \rho_{t} \rangle_{s} = \int_{0}^{t} dt_{2} \int_{0}^{t_{2}} dt_{1} \int d^{d}x_{1} \int d^{d}x_{2} \left[\hat{\mathbf{L}}^{U}(\mathbf{x}_{2}) G(\mathbf{x}_{2}, t_{2} - t_{1} | x_{1}) V(\mathbf{x}_{1}) + V(\mathbf{x}_{2}) G(\mathbf{x}_{2}, t_{2} - t_{1} | x_{1}) \mathbf{L}_{U}(\mathbf{x}_{1}) \right] p_{s}(\mathbf{x}_{1}) = \int_{0}^{t} dt_{2} \int_{0}^{t_{2}} dt_{1} \int d^{d}x_{1} \int d^{d}x_{2} \left[U(\mathbf{x}_{2}) \hat{\mathbf{j}}_{\mathbf{x}_{2}} G(\mathbf{x}_{2}, t_{2} - t_{1} | \mathbf{x}_{1}) V(\mathbf{x}_{1}) \right. \left. + V(\mathbf{x}_{2}) G(\mathbf{x}_{2}, t_{2} - t_{1} | \mathbf{x}_{1}) [U(\mathbf{x}_{1}) \hat{\mathbf{j}}_{\mathbf{x}_{1}} - \mathbf{D} \nabla_{\mathbf{x}_{1}} U(\mathbf{x}_{1})] \right] p_{s}(\mathbf{x}_{1}).$$
(29)

We note that for any function f the following identity holds

$$\int_{0}^{t} \mathrm{d}t_{2} \int_{0}^{t_{2}} \mathrm{d}t_{1} f(t_{2} - t_{1}) = \int_{0}^{t} \mathrm{d}t'(t - t') f(t'), \tag{30}$$

and further introduce the shorthand notation

$$\hat{\mathcal{I}}_{\mathbf{xy}}^{t}[\cdots] = \int_{0}^{t} \mathrm{d}t'(t-t') \int \mathrm{d}^{d}x_{1} \int \mathrm{d}^{d}x_{2} U(\mathbf{x}_{1}) V(\mathbf{x}_{2})[\cdots].$$
(31)

Moreover, we define $P_{\mathbf{y}}(\mathbf{x},t) \equiv G(\mathbf{x},t|\mathbf{y})p_{s}(\mathbf{y})$ and introduce the dual-reversed current operator $\hat{\mathbf{j}}_{\mathbf{x}}^{\dagger} \equiv \mathbf{j}_{s}(\mathbf{x})/p_{s}(\mathbf{x}) + \mathbf{D}p_{s}(\mathbf{x})\nabla_{\mathbf{x}}p_{s}^{-1}(\mathbf{x})$ which corresponds to $-\hat{\mathbf{j}}_{\mathbf{x}}^{\mathbf{j}_{s}\to-\mathbf{j}_{s}}$ [23]. With these notations, performing an integration by parts, and by relabeling $\mathbf{x}_{1} \leftrightarrow \mathbf{x}_{2}$ in one term, we rewrite Eq. (29) to obtain for the correlation

$$\langle \mathbf{J}_{t} \rho_{t} \rangle_{\mathrm{s}} - \langle \mathbf{J}_{t} \rangle \langle \rho_{t} \rangle_{\mathrm{s}} = \hat{\mathcal{I}}_{\mathbf{xy}}^{t} \Big[\hat{\mathbf{j}}_{\mathbf{x}_{1}} P_{\mathbf{x}_{2}}(\mathbf{x}_{1}, t') + \mathbf{j}_{\mathrm{s}}(\mathbf{x}_{1}) p_{\mathrm{s}}^{-1}(\mathbf{x}_{1}) P_{\mathbf{x}_{1}}(\mathbf{x}_{2}, t') + \mathbf{D} p_{\mathrm{s}}(\mathbf{x}_{1}) \nabla_{\mathbf{x}_{1}} p_{\mathrm{s}}(\mathbf{x}_{1})^{-1} P_{\mathbf{x}_{1}}(\mathbf{x}_{2}, t') \Big] - \langle \mathbf{J}_{t} \rangle \langle \rho_{t} \rangle_{\mathrm{s}} = \hat{\mathcal{I}}_{\mathbf{xy}}^{t} \Big[\hat{\mathbf{j}}_{\mathbf{x}_{1}} P_{\mathbf{x}_{2}}(\mathbf{x}_{1}, t') + \hat{\mathbf{j}}_{\mathbf{x}_{1}}^{\dagger} P_{\mathbf{x}_{1}}(\mathbf{x}_{2}, t') - 2 \mathbf{j}_{\mathrm{s}}(\mathbf{x}_{1}) p_{\mathrm{s}}(\mathbf{x}_{2}) \Big] .$$
(32)

We will discuss this result below, but first derive analogous results for (co)variances of densities and currents.

Instead of obtaining $\langle \rho_t^2 \rangle_s$ from the v^2 order in Eq. (27) we here consider a generalization to two densities, $\rho_t = \int_0^t V(\mathbf{x}_\tau) d\tau$ and $\rho'_t = \int_0^t U(\mathbf{x}_\tau) d\tau$. The Laplace-transformed tilted generator in Eq. (22) with Laplace variables v, v' corresponding to ρ_t, ρ'_t is obtained equivalently and gives $\hat{\mathcal{L}}(\mathbf{x}, v, v') = \hat{\mathcal{L}}(\mathbf{x}) - vV(\mathbf{x}) - v'U(\mathbf{x})$. The relative term in the Dyson series (by an adaption of Eq. (27) including v'U) becomes $[vV(\mathbf{x}_2) + v'U(\mathbf{x}_2)]G(\mathbf{x}_2, t_2 - t_1|\mathbf{x}_1)[vV(\mathbf{x}_1) + v'U(\mathbf{x}_1)]p_s(\mathbf{x}_1)$ (see also [26]). From this we obtain the known result [26, 1],

$$\left\langle \rho_t \rho_t' \right\rangle_{\rm s} - \left\langle \rho_t \right\rangle_{\rm s} \left\langle \rho_t' \right\rangle_{\rm s} = \hat{\mathcal{I}}_{\mathbf{x}\mathbf{y}}^t [P_{\mathbf{x}_2}(\mathbf{x}_1, t') + P_{\mathbf{x}_1}(\mathbf{x}_2, t') - 2p_{\rm s}(\mathbf{x}_1)p_{\rm s}(\mathbf{x}_2)].$$
(33)

For U = V this becomes the variance of ρ_t .

To obtain the current covariance, we accordingly require a tilted generator with two Fourier variables $\boldsymbol{\omega}, \boldsymbol{\omega}'$ corresponding to $\mathbf{J}_t = \int_{\tau=0}^{\tau=t} U(\mathbf{x}_{\tau}) \circ d\mathbf{x}_{\tau}$ and $\mathbf{J}'_t = \int_{\tau=0}^{\tau=t} V(\mathbf{x}_{\tau}) \circ d\mathbf{x}_{\tau}$, which can, by the same formalism, be derived as

$$\hat{\mathcal{L}}(\mathbf{x},\boldsymbol{\omega},\boldsymbol{\omega}') = \hat{L}(\mathbf{x}) - \mathrm{i}\boldsymbol{\omega}^T \cdot \hat{\mathbf{L}}^U(\mathbf{x}) - \mathrm{i}\boldsymbol{\omega}'^T \cdot \hat{\mathbf{L}}^V(\mathbf{x}) - U(\mathbf{x})^2 \boldsymbol{\omega}^T \mathbf{D}\boldsymbol{\omega} - V(\mathbf{x})^2 \boldsymbol{\omega}'^T \mathbf{D}\boldsymbol{\omega}' - 2U(\mathbf{x})V(\mathbf{x})\boldsymbol{\omega}^T \mathbf{D}\boldsymbol{\omega}' \hat{\mathbf{L}}^V(\mathbf{x}) \equiv V(\mathbf{x})\hat{\mathbf{j}}_{\mathbf{x}} - \mathbf{D}\nabla_{\mathbf{x}}V(\mathbf{x}).$$
(34)

The Dyson series (by adapting Eq. (27)) based on $\hat{\mathcal{L}}(\mathbf{x}, \boldsymbol{\omega}, \boldsymbol{\omega}')$ for two currents \mathbf{J}, \mathbf{J}' reads

$$\widetilde{\mathcal{P}}_{t}^{\mathbf{J}\mathbf{J}'}(\boldsymbol{\omega},\boldsymbol{\omega}'|p_{s}) = 1 + \int \mathrm{d}^{d}x_{1} \int_{0}^{t} \mathrm{d}t_{1} \left[\mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}'^{T} \cdot \hat{\mathbf{L}}^{V}(\mathbf{x}_{1}) + 2U(\mathbf{x}_{1})V(\mathbf{x}_{1})\boldsymbol{\omega}^{T}\mathbf{D}\boldsymbol{\omega}' \right] p_{s}(\mathbf{x}_{1}) \\
+ \int \mathrm{d}^{d}x_{1} \int \mathrm{d}^{d}x_{2} \int_{0}^{t} \mathrm{d}t_{2} \int_{0}^{t_{2}} \mathrm{d}t_{1} \left[\mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{2}) + \mathrm{i}\boldsymbol{\omega}'^{T} \cdot \hat{\mathbf{L}}^{V}(\mathbf{x}_{2}) \right] \\
G(\mathbf{x}_{2}, t_{2} - t_{1}|\mathbf{x}_{1}) \left[\mathrm{i}\boldsymbol{\omega}^{T} \cdot \hat{\mathbf{L}}^{U}(\mathbf{x}_{1}) + \mathrm{i}\boldsymbol{\omega}'^{T} \cdot \hat{\mathbf{L}}^{V}(\mathbf{x}_{1}) \right] p_{s}(\mathbf{x}_{1}) + O(\boldsymbol{\omega}^{2}, \boldsymbol{\omega}'^{2}).$$
(35)

The expectation value of the product of current components $\langle J_{t,n}J'_{t,m}\rangle_{\rm s}$ is given by the terms that are linear in $\omega_n\omega'_m$, i.e. (recall $D_{nm} = D_{mn}$)

$$\left\langle J_{t,n}J_{t,m}' \right\rangle_{\rm s} = 2tD_{nm} \int \mathrm{d}^{d}x_{1} U(\mathbf{x}_{1})V(\mathbf{x}_{1})p_{\rm s}(\mathbf{x}_{1}) + \int_{0}^{t} \mathrm{d}t'(t-t') \int \mathrm{d}^{d}x_{1} \int \mathrm{d}^{d}x_{2} \\ \left[\hat{L}_{n}^{U}(\mathbf{x}_{2})G(\mathbf{x}_{2},t'|\mathbf{x}_{1}) \cdot \hat{L}_{m}^{V}(\mathbf{x}_{1})p_{\rm s}(\mathbf{x}_{1}) + \hat{L}_{m}^{V}(\mathbf{x}_{2})G(\mathbf{x}_{2},t'|\mathbf{x}_{1}) \cdot \hat{L}_{n}^{U}(\mathbf{x}_{1})p_{\rm s}(\mathbf{x}_{1}) \right].$$
(36)

We denote by $\hat{=}$ equality up to gradient terms that vanish upon integration to write

$$\hat{L}_{n}^{U}(\mathbf{x}_{2})G(\mathbf{x}_{2},t'|\mathbf{x}_{1}) \cdot \hat{L}_{m}^{V}(\mathbf{x}_{1})p_{s}(\mathbf{x}_{1}) = U(\mathbf{x}_{2})\hat{\mathbf{j}}_{\mathbf{x}_{2},n}G(\mathbf{x}_{2},t'|\mathbf{x}_{1}) \times \\
\left[V(\mathbf{x}_{1})\mathbf{j}_{s}(\mathbf{x}_{1})p_{s}^{-1}(\mathbf{x}_{1}) - p_{s}(\mathbf{x}_{1})\mathbf{D}\nabla_{\mathbf{x}_{1}}p_{s}(\mathbf{x}_{1})^{-1} - \mathbf{D}\nabla_{\mathbf{x}_{1}}V(\mathbf{x}_{1})\right]_{m}p_{s}(\mathbf{x}_{1}) \\
= U(\mathbf{x}_{2})V(\mathbf{x}_{1})\hat{\mathbf{j}}_{\mathbf{x}_{2},n}[\mathbf{j}_{s}(\mathbf{x}_{1})p_{s}^{-1}(\mathbf{x}_{1}) + p_{s}(\mathbf{x}_{1})\mathbf{D}\nabla_{\mathbf{x}_{1}}p_{s}^{-1}(\mathbf{x}_{1})]_{m}G(\mathbf{x}_{2},t'|\mathbf{x}_{1})p_{s}(\mathbf{x}_{1}) \\
= U(\mathbf{x}_{2})V(\mathbf{x}_{1})\hat{\mathbf{j}}_{\mathbf{x}_{2},n}\hat{\mathbf{j}}_{\mathbf{x}_{1},m}^{\dagger}P_{\mathbf{x}_{1}}(\mathbf{x}_{2},t).$$
(37)

Inserting this into Eq. (36), and relabeling in one term $\mathbf{x}_1 \leftrightarrow \mathbf{x}_2$ we obtain for the *nm*-element of the current covariance matrix

$$\left\langle J_{t,n}J'_{t,m}\right\rangle_{\mathbf{s}} - \left\langle J_{t,n}\right\rangle_{\mathbf{s}} \left\langle J'_{t,m}\right\rangle_{\mathbf{s}} = 2tD_{nm} \int \mathrm{d}^{d}x_{1} U(\mathbf{x}_{1})V(\mathbf{x}_{1})p_{\mathbf{s}}(\mathbf{x}_{1}) + \hat{\mathcal{I}}^{t}_{\mathbf{xy}} \left[\hat{\mathbf{j}}_{\mathbf{x}_{1},n}\hat{\mathbf{j}}^{\dagger}_{\mathbf{x}_{2},m}P_{\mathbf{x}_{2}}(\mathbf{x}_{1},t') + \hat{\mathbf{j}}_{\mathbf{x}_{2},m} \cdot \hat{\mathbf{j}}^{\dagger}_{\mathbf{x}_{1},n}P_{\mathbf{x}_{1}}(\mathbf{x}_{2},t')\right].$$
(38)

This result for the current covariance matrix and Eq. (32) for the current-density correlation are the natural generalizations of the density-density covariance Eq. (33), as described in detail in Refs. [22, 23], with the additional $2tD_{nm}$ -term in Eq. (38) arising from the $(\mathbf{dW}_{\tau})^2$ contribution in $J_{t,n}J'_{t,m}$. While the density-density covariance Eq. (33) only depends on integration over all paths from \mathbf{x}_1 to \mathbf{x}_2 (and vice versa) in time t' via $P_{\mathbf{x}_1}(\mathbf{x}_2, t')$, the current-density correlation Eq. (32) instead involves $\hat{\mathbf{j}}_{\mathbf{x}_1}P_{\mathbf{x}_2}(\mathbf{x}_1, t')$ and $\hat{\mathbf{j}}_{\mathbf{x}_1}^{\ddagger} P_{\mathbf{x}_1}(\mathbf{x}_2, t')$ which describe currents at the final- and initial-points, respectively [23]. This notion is further extended in the result Eq. (38) where $\hat{\mathbf{j}}_{\mathbf{x}_2,m} \hat{\mathbf{j}}_{\mathbf{x}_1,n}^{\ddagger} P_{\mathbf{x}_1}(\mathbf{x}_2, t')$ corresponds to products of components of displacements along individual trajectories from \mathbf{x}_1 to \mathbf{x}_2 [22]. Together with the results in [22, 23] derived directly from Itô calculus (thus avoiding Feynman-Kac tilting), the present results provide three independent but equivalent general methods for studying the fluctuations and correlations of dynamical functionals in Eq. (5).

4. Conclusion

We employed a Feynman-Kac approach to derive moments and correlations of dynamical functionals of diffusive paths — the time-integrated densities and currents. We presented two different but equivalent approaches to tilting the generator — Itô and functional calculus. Our results place the different approaches to the statistics of dynamical functionals employed in the field on a common footing, and we hope that they will contribute to connecting the often virtually disjoint communities working on very similar problems with distinct methods. Moreover, these results may have important implications for large deviation theory and stochastic thermodynamics, in particular for the physical and mathematical role of coarse graining as discussed in [22, 23].

Acknowledgments

Financial support from Studienstiftung des Deutschen Volkes (to C. D.) and the German Research Foundation (DFG) through the Emmy Noether Program GO 2762/1-2 (to A. G.) is gratefully acknowledged.

References

- [1] M. Kac, "On distributions of certain Wiener functionals," Trans. Am. Math. Soc. 65 (1949) 1.
- [2] D. A. Darling and M. Kac, "On occupation times for Markoff processes," Trans. Am. Math. Soc. 84 (1957) 444.
- [3] E. Aghion, D. A. Kessler, and E. Barkai, "From non-normalizable Boltzmann-Gibbs statistics to infinite-ergodic theory," *Phys. Rev. Lett.* **122** (2019) 010601.
- [4] S. Carmi and E. Barkai, "Fractional Feynman-Kac equation for weak ergodicity breaking," *Phys. Rev. E* 84 (2011) 061104.
- [5] S. N. Majumdar and A. Comtet, "Local and occupation time of a particle diffusing in a random medium," *Phys. Rev. Lett.* 89 (2002) 060601.
- [6] 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.
- [7] S. N. Majumdar, "Brownian functionals in physics and computer science," Curr. Sci. 89 (2005) 2075.
- [8] A. J. Bray, S. N. Majumdar, and G. Schehr, "Persistence and first-passage properties in nonequilibrium systems," Adv. Phys. 62 (2013) 225.
- [9] G. Bel and E. Barkai, "Weak ergodicity breaking in the continuous-time random walk," *Phys. Rev. Lett.* 94 (2005) 240602.

- [10] C. Maes, K. Netočný, and B. Wynants, "Steady state statistics of driven diffusions," *Phys. A* 387 (2008) 2675.
- [11] H. Touchette, "The large deviation approach to statistical mechanics," Phys. Rep. 478 (2009) 1.
- [12] S. Kusuoka, K. Kuwada, and Y. Tamura, "Large deviation for stochastic line integrals as L^p -currents," *Probab. Theory Relat. Fields* 147 (2009) 649.
- [13] R. Chetrite and H. Touchette, "Nonequilibrium microcanonical and canonical ensembles and their equivalence," *Phys. Rev. Lett.* **111** (2013) 120601.
- [14] R. Chetrite and H. Touchette, "Nonequilibrium Markov processes conditioned on large deviations," *Annales Henri Poincaré* 16 (2014) 2005.
- [15] A. C. Barato and R. Chetrite, "A formal view on level 2.5 large deviations and fluctuation relations," J. Stat. Phys. 160 (2015) 1154.
- [16] 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.
- [17] H. Touchette, "Introduction to dynamical large deviations of Markov processes," *Phys. A* 504 (2018) 5.
- [18] 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.
- [19] 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.
- [20] A. Dechant and S.-i. Sasa, "Improving thermodynamic bounds using correlations," *Phys. Rev. X* 11 (2021) 041061.
- [21] A. Dechant and S.-i. Sasa, "Continuous time reversal and equality in the thermodynamic uncertainty relation," *Phys. Rev. Research* 3 (2021) 042012.
- [22] C. Dieball and A. Godec, "Mathematical, thermodynamical, and experimental necessity for coarse graining empirical densities and currents in continuous space," (2022), arXiv:2105.10483 [cond-mat.stat-mech].
- [23] C. Dieball and A. Godec, "Coarse graining empirical densities and currents in continuous-space steady states," (2022), arXiv:2204.06553 [cond-mat.stat-mech].
- [24] A. Rebenshtok and E. Barkai, "Weakly non-ergodic statistical physics," J. Stat. Phys. 133 (2008) 565.
- [25] 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.
- [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] F. Coghi, R. Chetrite, and H. Touchette, "Role of current fluctuations in nonreversible samplers," *Phys. Rev. E* 103 (2021) 062142.
- [28] U. Seifert, "Stochastic thermodynamics: From principles to the cost of precision," Phys. A 504 (2018) 176.
- [29] T. Koyuk and U. Seifert, "Thermodynamic uncertainty relation for time-dependent driving," *Phys. Rev. Lett.* **125** (2020) 260604.
- [30] P. Pietzonka, A. C. Barato, and U. Seifert, "Universal bounds on current fluctuations," *Phys. Rev. E* 93 (2016) 052145.
- [31] U. Seifert, "Entropy production along a stochastic trajectory and an integral fluctuation theorem," *Phys. Rev. Lett.* **95** (2005) 040602.
- [32] S. Pigolotti, I. Neri, É. Roldán, and F. Jülicher, "Generic properties of stochastic entropy production," *Phys. Rev. Lett.* **119** (2017) 140604.
- [33] U. Seifert, "Stochastic thermodynamics, fluctuation theorems and molecular machines," Rep. Prog. Phys. 75 (2012) 126001.
- [34] G. Dell'Antonio, "Lecture 6: Lie-Trotter formula, Wiener process, Feynman-Kac formula,"

Lectures on the Mathematics of Quantum Mechanics II: Selected Topics (2016) 133.

- [35] G. C. M. A. Ehrhardt, S. N. Majumdar, and A. J. Bray, "Persistence exponents and the statistics of crossings and occupation times for Gaussian stationary processes," *Phys. Rev. E* 69 (2004) 016106.
- [36] S. Sabhapandit, S. N. Majumdar, and A. Comtet, "Statistical properties of functionals of the paths of a particle diffusing in a one-dimensional random potential," *Phys. Rev. E* 73 (2006) 051102.
- [37] 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.
- [38] 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.
- [39] 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.
- [40] N. Ikeda and S. Watanabe, Stochastic Differential Equations and Diffusion Processes. North Holland, 1st edition ed., 1981. eBook ISBN: 9780080960128.
- [41] R. F. Fox, "Functional-calculus approach to stochastic differential equations," Phys. Rev. A 33 (1986) 467.
- [42] R. F. Fox, "Stochastic calculus in physics," J. Stat. Phys. 46 (1987) 1145.
- [43] H. Risken, The Fokker-Planck Equation. Springer Berlin Heidelberg, 1989.
- [44] C. W. Gardiner, Handbook of stochastic methods for physics, chemistry, and the natural sciences. Springer-Verlag, Berlin New York, 1985.
- [45] A. Lapolla and A. Godec, "Unfolding tagged particle histories in single-file diffusion: exact singleand two-tag local times beyond large deviation theory," New J. Phys. 20 (2018) 113021.
- [46] L. F. Cugliandolo, V. Lecomte, and F. van Wijland, "Building a path-integral calculus: a covariant discretization approach," J. Phys. A: Math. Theor. 52 (2019) 50LT01.