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 usually studied within the Feynman-Kac tilting formalism, which in the Physics literature is typically derived by some form of Kramers-Moyal expansion, or in the Mathematical literature via the Cameron-Martin-Girsanov approach. Here we derive the Feynman-Kac theory for general additive dynamical functionals directly via Itô calculus and via functional calculus, where the latter results 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 recently in Dieball and Godec (2022 Phys. Rev. Lett. 129 140601) and Dieball and Godec (2022 Phys. Rev. Res. 4 033243). We hope for our work to put the different approaches to the statistics of dynamical functionals employed in the field on a common footing, and to illustrate more easily accessible ways to the tilting formalism.

1. Introduction

Dynamical functionals and diverse path-based observables [1–8], such as local and occupation times (also known as the “empirical density”) [9–17] as well as diverse time-integrated and time-averaged currents [18–31] are central to “time-average statistical mechanics” [32–34], large deviation theory (see e.g. [19, 22, 25, 26, 35]), macroscopic fluctuation theory [36–38], and path-wise, stochastic thermodynamics [28, 29, 39–44].

Several techniques are available for the study of dynamical functionals, presumably best known is the Lie-Trotter-Kato formalism [10, 45] that was employed by Kac in his seminal work [9]. The techniques typically employed in physics rely on an analogy to quantum mechanical problems (see e.g. [15]) or assume some form of the Kramers-Moyal expansion [13, 16, 46, 47] (see also interesting generalizations to anomalous dynamics [12, 17]).

Deriving Feynman-Kac theory [9] of such additive functionals amounts to obtaining a “tilted” generator which generates the time-evolution of the observables under consideration. The tilted evolution operator can be obtained using the Cameron-Martin-
Girsanov theorem [48, 49] — a well-known technical theorem often employed in the Mathematical Physics literature [21–23].

In this paper we develop the Itô [34,50] and functional calculus [51,52] approaches to Feynman-Kac theory, whereby we a focus on the methodology and accessibility for readers that are unfamiliar with the Cameron-Martin-Girsanov approach to “tilting”. We thereby hope to provide two accessible alternative (but equivalent) ways to obtaining the tilted generator. While the Itô approach already exists (see e.g. [34] for the empirical density), our functional calculus approach is a generalization of the pedagogical work of Fox [51,52] and is aimed towards readers who prefer to avoid Itô calculus. Since both methods are equivalent they yield the same tilted generator. This generator is subsequently used to re-derive recent results on the statistics of time-integrated densities and currents obtained in References [30,31] using a different, more direct, stochastic calculus approach that avoids tilting. In particular, these results illustrate the use of the tilted generator to derive the statistics of time-integrated observables for finite times, i.e. extending beyond large deviation theory.

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 [51,52] we derive in Sec. 2.3 the 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

In this section, we first introduce the considered stochastic dynamics and define what we call “dynamical functionals”. Subsequently we derive the tilted generator (i.e. the operator generating the time-evolution of time-integrated functionals) based on Itô calculus, and finally equivalently also via functional calculus.

2.1. Set-Up

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

$$\text{d}x_t = F(x_t)\text{d}t + \sigma \text{d}W_t, \quad (1)$$

where $\text{d}W_t$ is denotes increment of the Wiener process [50]. The corresponding diffusion constant is $D = \sigma \sigma^T / 2$. For simplicity we stick to additive noise whereas all present results generalize to multiplicative noise $D(x)$ as described in [31]. In the physics literature Eq. (1) is typically written in the form of a Langevin equation

$$\dot{x}_t = F(x_t) + f(t), \quad (2)$$
with white noise amplitude $\langle f(t)f(t')^T \rangle = 2D\delta(t-t')$. Comparing the two equations, $f(t)$ corresponds to the derivative of $W_t$, which however (with probability one) is not differentiable; more precisely, upon taking $dt \to 0$ one has $||dW_t/dt|| = \infty$ 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

$$\hat{L}(x) = -\nabla_x \cdot F(x) + \nabla_x \cdot D \nabla_x = -\nabla_x \cdot \hat{j}_x,$$

where we have defined the current operator $\hat{j}_x \equiv F(x) - D \nabla_x$. Note that all differential operators act on all functions to the right, e.g. $\nabla_x \cdot F(x)g(x) = g(x)\nabla_x \cdot F(x) + F(x) \cdot \nabla_x g(x)$. Although the approach presented here is more general, we restrict our attention to (possibly non-equilibrium) steady states where the drift $F(x)$ is sufficiently smooth and confining to assure the existence of a steady-state (invariant) density $p_s(x) = \lim_{t \to \infty} G(x,t|x_0)$ and steady-state current $j_s(x) = \hat{j}_x p_s(x)$. The special case $j_s(x) = 0$ corresponds to equilibrium steady states. For systems that eventually evolve into a steady state we can rewrite the current operator as [31] (again the differential operator in $\nabla_x p_s^{-1}(x)$ also acts on functions to the right if $\hat{j}_x$ is applied to a function)

$$\hat{j}_x = j_s(x)p_s^{-1}(x) - Dp_s(x)\nabla_x p_s^{-1}(x).$$

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

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

$$J_t = \int_0^t U(x_\tau') \circ dx_\tau$$

$$\rho_t = \int_0^t V(x_\tau) d\tau,$$

with differentiable and square-integrable (real-valued) functions $U, V : \mathbb{R}^d \to \mathbb{R}$ and $\circ$ denoting the Stratonovich integral [50, 55, 56]. These objects depend on the whole trajectory $[x_\tau]_{0 \leq \tau \leq t}$ 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 $x_t, \rho_t, J_t$ 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 $\rho_t/t$ (under the term of local/occupation time fraction) [9, 34, 57]. 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 [22, 23] (in this case obtained via the Feynman-Kac-Girsanov approach).
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 $dU(x_r)dx_r/2$ and $dx_rdx^T_r = 2Dd\tau$ (where $D = \sigma\sigma^T/2$) we obtain from Eqs. (1) and (5) the increments (curly brackets $\{\nabla \ldots\}$ throughout denote that derivatives only act inside brackets)

$$
\begin{align*}
\text{d}J_\tau &= U(x_r) \circ \text{d}x_r = U(x_r)dx_r + D\{\nabla_x U\}(x_r)\text{d}\tau \\
\text{d}\rho_\tau &= V(x_r)\text{d}\tau.
\end{align*}
$$

(6)

We use Itô’s Lemma [50] in $d$ dimensions for a twice differentiable test function $f = f(x_t, \rho_t, J_t)$ and Eqs. (1) and (6), to obtain

$$
\text{d}f = \sum_{i=1}^{d} \frac{\partial f}{\partial x^i} \text{d}x^i_t + \sum_{i=1}^{d} \frac{\partial f}{\partial \rho} \text{d}\rho_t + \sum_{i=1}^{d} \frac{\partial f}{\partial J^i} \text{d}J^i_t \\
+ \frac{1}{2} \sum_{i,j=1}^{d} \left( \frac{\partial^2 f}{\partial x^i_t \partial x^j} \text{d}x^i_t \text{d}x^j_t + \frac{\partial^2 f}{\partial J^i_t \partial J^j} \text{d}J^i_t \text{d}J^j_t + 2 \frac{\partial^2 f}{\partial x^i_t \partial J^j} \text{d}x^i_t \text{d}J^j_t \right)
$$

$$
= \left[ (\nabla_x f) + (\nabla J f)U(x_t) \right][F(x_t)dt + \sigma dW_t] + (\nabla J f)D\{\nabla_x U\}(x_t)dt + V(x_t)\partial_\rho f dt
+ (\nabla_x^T D V_x + U(x_t)^2 \nabla_{\nabla J}^T D \nabla_j + 2U(x_t)\nabla_x^T D \nabla_j) f dt.
$$

(7)

For the time derivative of $f$ this gives

$$
\frac{d}{dt} f(x_t, \rho_t, J_t) = \left[ F + \sigma \frac{dW_t}{dt} \right] (\nabla_x + U \nabla J)
+ V \partial_\rho + \nabla_x^T D \nabla_x + U^2 \nabla_{\nabla J}^T D \nabla_j + 2U \nabla_x^T D \nabla_j \right] f(x_t, \rho_t, J_t).
$$

(8)

Following this formalism, we move towards a tilted Fokker-Planck equation [9, 34]. Using the conditional probability density $Q_t(x, \rho, J|x_0)$ we may write (omitting $x$ dependence in $F, U, V$ for brevity) the evolution equation for $\langle f(x_t, \rho_t, J_t)\rangle_{x_0}$, i.e. the expected value of $f(x_t, \rho_t, J_t)$ over the ensemble of paths propagating between $x_0$ and $x$ in time $t$. Using Eq. (8) and integration by parts, we obtain (note that non-negative functions $V \geq 0$ imply $\rho \geq 0$, such that one would restrict the $\rho$-integration to $\int_0^{\infty} d\rho$ as in Ref. [34])

$$
\begin{align*}
\frac{d}{dt} \langle f(x_t, \rho_t, J_t)\rangle_{x_0} &= \int d^dx \int_{-\infty}^{\infty} d\rho \int d^dJ f(x, \rho, J)\partial_t Q_t(x, \rho, J|x_0) \\
= \int d^dx \int_{-\infty}^{\infty} d\rho \int d^dJ Q_t(x, \rho, J|x_0) \left[ F(\nabla_x + U \nabla J) + \{\nabla_x U\}D \nabla_j + V \partial_\rho + \nabla_x^T D \nabla_x + U^2 \nabla_{\nabla J}^T D \nabla_j + 2U \nabla_x^T D \nabla_j \right] f(x, \rho, J)
+ \nabla_x^T D \nabla_x + U^2 \nabla_{\nabla J}^T D \nabla_j + 2U \nabla_x^T D \nabla_j \right] Q_t(x, \rho, J|x_0).
\end{align*}
$$

(9)
Since the test function \( f \) is an arbitrary twice differentiable function, the resulting tilted Fokker-Planck equation reads

\[
\partial_t Q_t(x, \rho, J|x_0) = \hat{L}_{x, \rho, J} Q_t(x, \rho, J|x_0),
\]

with the tilted Fokker-Planck operator \( \hat{L}_{x, \rho, J} \)

\[
\hat{L}_{x, \rho, J} = -\nabla_x \cdot F(x) + \nabla_x^T D \nabla_x - V(x) \partial_\rho - U(x) F(x) \cdot \nabla J
\]

\[
- \{ \nabla_x U(x) \}^T D \nabla J + U(x)^2 \nabla J^T D \nabla J + 2 \nabla J^T D \nabla_x U(x)
\]

\[
= - [\nabla_x + U(x) \nabla J] F(x) - V(x) \partial_\rho + [\nabla_x + U(x) \nabla J]^T D [\nabla_x + U(x) \nabla J].
\]  

(11)

We see that the \( \rho \) dependence enters in standard Feynman-Kac form [9,34], whereas the \( J \) dependence enters less trivially and shifts the gradient operator \( \nabla_x \rightarrow \nabla_x + U(x) \nabla J \).

2.3. Tilting via functional calculus

We now re-derive the tilted Fokker-Planck operator in Eq. (11) using a functional calculus approach [51,52] instead of the Itô calculus in the previous section. This shows that both alternative approaches are equivalent, as expected. We closely follow the derivation of the Fokker-Planck equation in reference [51] but for \( d \)-dimensional space and we generalize the approach to include the functionals defined in Eq. (5). The following approach is equivalent to a Stratonovich interpretation of stochastic calculus which is manifested in the convention \( \int_0^t \delta(t')dt' = \int_0^t \delta(t-t')dt' = 1/2 \) [51]. The white noise term \( f(\tau) \) with \( \langle f(\tau)f(\tau') \rangle_s = 2D \delta(\tau - \tau') \) in the Langevin equation (2) can be considered to be described by a path-probability measure [51]

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

(12)

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

We now derive a tilted Fokker-Planck equation for the joint conditional density \( Q \) of \( x_t \) and the functionals \( J_t, \rho_t \), as defined in Eq. (5), given a deterministic initial condition \( x_0 \) at time \( t = 0 \),

\[
Q_t(x, \rho, J|x_0) \equiv \int Df P[f] \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t).
\]

(13)

Note for the time derivatives that \( J_t = U(x_t)x_t \) and \( \rho_t = V(x_t) \) to obtain (as a \( \delta \) For non-negative functions \( V \geq 0 \) an additional boundary term appears at \( \rho = 0 \) upon partial integration in Eq. (9), leading to an extra term \( -V(x) \delta(\rho) \) in Eq. (10) that ensures conservation of probability (see [34]).
generalization of the calculation in reference [51] to dynamical functionals)
\[ \partial_t Q(x, \rho, J, t | x_0) = \partial_t \int \mathcal{D}f P[f] \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) \]
\[ = \int \mathcal{D}f P[f] \left[ -\nabla \cdot \dot{x}_t - \partial_\rho \dot{\rho}_t - \nabla J \cdot \dot{J}_t \right] \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) \]
\[ = \int \mathcal{D}f P[f] \left[ -\nabla \cdot [F(x_t) + f(t)] - V(x_t) \partial_\rho - U(x_t) [F(x_t) + f(t)] \nabla J \right] \times \]
\[ \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) \]
\[ = \left[ -\nabla_x F(x) - V(x) \partial_\rho - U(x) F(x) \nabla J \right] Q_t(x, \rho, J | x_0) \]
\[ - \left[ \nabla_x + U(x) \nabla J \right] \cdot \int \mathcal{D}f P[f] f(t) \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t). \] (14)

The functional derivative of Eq. (12) reads [51]
\[ \frac{\delta P[f]}{\delta f(t)} = -\frac{1}{2} D^{-1} f(t) P[f], \] (15)

which we use to obtain, via an integration by parts in \( \delta f(t) \),
\[ - \int \mathcal{D}f P[f] f(t) \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) \]
\[ = 2D \int \mathcal{D}f \frac{\delta P[f]}{\delta f(t)} \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) \]
\[ = -2D \int \mathcal{D}f P[f] \frac{\delta}{\delta f(t)} \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t). \] (16)

As before, differentials are understood to act on all functions to the right, i.e. \( \frac{\delta}{\delta f(t)} \) here acts on the full product of delta functions. We obtain
\[ \frac{\delta}{\delta f(t)} \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) \]
\[ = \left[ -\nabla_x \frac{\delta x_t}{\delta f(t)} - \partial_\rho \frac{\delta \rho_t}{\delta f(t)} - \nabla J \frac{\delta x_t}{\delta f(t)} \right] \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t), \] (17)

and we use that \( \delta \rho_t / \delta f(t) = 0 \), and \( \delta x_t / \delta f(t) = 1/2 \) [51] which implies \( \delta J_t / \delta f(t) = U(x_t) 1/2 \), to get
\[ \frac{\delta}{\delta f(t)} \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t) = \frac{1}{2} \left[ -\nabla_x - U(x_t) \nabla J \right] \delta(x - x_t) \delta(\rho - \rho_t) \delta(J - J_t). \] (18)

Plugging Eq. (18) first into Eq. (16) and then into Eq. (14) yields the tilted Fokker-Planck equation for the joint conditional density
\[ \partial_t Q_t(x, \rho, J | x_0) = \left[ -\nabla_x F(x) - V(x) \partial_\rho - U(x) F(x) \nabla J \right] \]
\[ + \left[ \nabla_x + U(x) \nabla J \right] D \left[ \nabla_x + U(x) \nabla J \right] Q_t(x, \rho, J | x_0). \] (19)

Note that Eq. (19) 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

In this section we employ the tilted Fokker-Planck equation (19) to derive results for the mean value and (co)variances of time-integrated densities and currents. These follow as derivatives of the characteristic function evaluated at zero, and it thus suffices to treat the tilt as a perturbation of the “bare” generator (see [34]). The derivation is based on a Dyson expansion of the exponential of a Fourier-transformed tilted generator (i.e. tilted Fokker-Planck operator). Therefore, consider a one-dimensional Fourier variable $\nu$ and a $d$-dimensional Fourier variable $\omega = (\omega_1, \ldots, \omega_d)$ and define the Fourier transform of $Q_t(x, \rho, J|x_0)$ as

$$\tilde{Q}_t(x, \nu, \omega|x_0) \equiv \int_{-\infty}^{\infty} d\rho \int d^dJ Q_t(x, \rho, J|x_0) \exp \left( -i\nu \rho - i\omega \cdot J \right). \quad (20)$$

In the case $V \geq 0$ where $\rho \geq 0$ one would instead take the Laplace transform in the $\rho$-coordinate, see Ref. [34]. Recall the (untilted) Fokker-Planck operator $\hat{L}(x) = -\nabla_x \cdot \hat{j}_x$ with the current operator $\hat{j}_x = F(x) - D \nabla_x$ from Eq. (3). The Fourier transform of the tilted Fokker-Planck operator in Eqs. (11) and (19) reads

$$\hat{L}(x, \nu, \omega) = \hat{L}(x) - i\nu V(x) - i\omega^T \cdot \hat{L}^U(x) - U(x) \omega^T D \omega,$$

$$\hat{L}^U(x) \equiv U(x) \hat{j}_x - D \nabla_x U(x). \quad (21)$$

As always, the differential operators act on all functions to the right unless written inside curly brackets, i.e. $\nabla_x U(x) = \{\nabla_x U(x)\} + U(x) \nabla_x$. Note that whereas we obtained the tilted generator directly and only subsequently Fourier transformed it, there are also approaches that directly target the Fourier image of the tilted generator (see e.g. [58]). Compared to the tilt of the density (i.e. the $\nu$-term; see also [34]), the tilt corresponding to the current observable ($\omega$-terms) involves more terms and even a term that is second order in $\omega$. The second order term occurs since $(dW_\tau)^2 \sim d\tau$ and therefore (in contrast to $d\tau dW_\tau$ and $d\tau^2$) 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. For the derivation of the moments of $\rho_t$ and $J_t$, we introduce and expand the characteristic function (also known as moment-generating function)

$$\tilde{P}_t^{\nu3}(\nu, \omega|p_s) \equiv \langle e^{-i\nu \rho_t - i\omega \cdot J_t} \rangle_s = 1 - i\nu \langle \rho_t \rangle_s - i\omega \cdot \langle J_t \rangle_s - \nu \omega \cdot \langle \rho_t J_t \rangle_s + O(\omega^2, \nu^2). \quad (22)$$

This expansion in $\nu, \omega$ will now be compared to the Dyson expansion of the exponential of Eq. (21) which yields expressions for $\langle \rho_t \rangle_s, \langle J_t \rangle_s, \langle \rho_t J_t \rangle_s$ by comparing individual orders.
The Dyson expansion allows to expand for small $|\nu|, |\omega|$ (see also [34])
\[
e^{\hat{L}(x,v,\omega)t} = 1 - i \int_0^t dt_1 e^{\hat{L}(x_1)(t-t_1)} \left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] e^{\hat{L}(x_1)t_1} \\
- \int_0^t dt_2 \int_0^{t_2} dt_1 e^{\hat{L}(x_1)(t-t_2)} \left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] e^{\hat{L}(x_1)(t_2-t_1)} \\
\left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] e^{\hat{L}(x_1)t_1} + O(\omega^2, \nu^2).
\] (23)

Using that the first propagation only differs from 1 by total derivatives (recall $\hat{L}(x) = -\nabla_x \cdot \hat{j}_x$), and using for the last propagation term $e^{\hat{L}(x_1)t_1} p_s(x_1) = p_s(x_1)$, we obtain
\[
\hat{P}^{\nu\omega}_t(v, \omega|p_s) = \int d^d x_1 e^{\hat{L}(x,v,\omega)t} p_s(x_1) \\
= 1 - i \int d^d x_1 \int_0^t dt_1 \left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] p_s(x_1) \\
- \sum_{l,m=1}^{d} \int d^d x_1 \int_0^t dt_2 \int_0^{t_2} dt_1 \left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] e^{\hat{L}(x_1)(t_2-t_1)} \\
\left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] p_s(x_1) + O(\omega^2, \nu^2).
\] (24)

We substitute the one-step propagation by the conditional density $G(x_2, t|x_1) = e^{\hat{L}(x_1)t} \delta(x_2 - x_1)$ [56, 59],
\[
\int d^d x_1 f(x_1) e^{\hat{L}(x_1)(t_2-t_1)} g(x_1) = \int d^d x_1 \int d^d x_2 f(x_2) G(x_2, t_2 - t_1|x_1) g(x_1),
\] (25)

which yields
\[
\hat{P}^{\nu\omega}_t(v, \omega|p_s) = 1 - i \int d^d x_1 \int_0^t dt_1 \left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] p_s(x_1) \\
- \int d^d x_1 \int d^d x_2 \int_0^t dt_2 \int_0^{t_2} dt_1 \left[ \nu V(x_2) + \omega^T \cdot \hat{L}(x_2) \right] \\
G(x_2, t_2 - t_1|x_1) \left[ \nu V(x_1) + \omega^T \cdot \hat{L}(x_1) \right] p_s(x_1) + O(\omega^2, \nu^2).
\] (26)

This concludes the expansion of the exponential of the Fourier transformed tilted generator. Now, by comparing the definition and expansion of the characteristic function Eq. (22) with the result Eq. (26) from the Dyson expansion, we obtain the moments and correlations of the functionals $J_t = \int_{\tau=t}^{\tau=t} U(x_\tau) \circ dx_\tau$ and $\rho_t = \int_0^t V(x_\tau) d\tau$.

Note that the first moments (i.e. the mean values for steady-state initial conditions) can also be obtained directly [18, 31] but we obtain them here by comparing the terms of order $\nu$ and $\omega$ in Eqs. (22) and (26),
\[
\langle \rho_t \rangle_s = \int_0^t dt_1 \int d^d x_1 V(x_1) p_s(x_1) = t \int d^d x_1 V(x_1) p_s(x_1) \\
\langle J_t \rangle_s = t \int d^d x_1 [U(x_1) \hat{j}_{x_1} - D \nabla_{x_1} U(x_1)] p_s(x_1) = t \int d^d x_1 U(x_1) \hat{j}_s(x_1),
\] (27)
where $\nabla_{x_1} U(x_1)p_s(x_1)$ vanishes after integration by parts and $\mathbf{j}_s(x_1) \equiv \hat{j}_x p_s(x_1)$ is the steady-state current.

By comparing the terms of order $\nu \omega$ in Eqs. (22) and (26) we have for the steady-state expectation $\langle \mathbf{J}_t \rho_t \rangle_s$ that

$$
\langle \mathbf{J}_t \rho_t \rangle_s = \int_0^t dt_2 \int_0^{t_2} dt_1 \int d^4x_1 \int d^4x_2 \left[ L^U(x_2)G(x_2,t_2 - t_1|x_1)V(x_1) + V(x_2)G(x_2,t_2 - t_1|x_1)L_U(x_1) \right] p_s(x_1)
$$

$$
= \int_0^t dt_2 \int_0^{t_2} dt_1 \int d^4x_1 \int d^4x_2 \left[ U(x_2)\hat{j}_{x_2} G(x_2,t_2 - t_1|x_1)V(x_1) + V(x_2)G(x_2,t_2 - t_1|x_1)U(x_1)\hat{j}_{x_1} - \mathbf{D} \nabla_{x_1} U(x_1) \right] p_s(x_1).
$$

(28)

We note that for any function $f$ the following identity holds

$$
\int_0^t dt_2 \int_0^{t_2} dt_1 f(t_2 - t_1) = \int_0^t dt' (t - t') f(t'),
$$

(29)

and further introduce the shorthand notation

$$
\hat{T}_{x_1y}[\cdots] = \int_0^t dt' (t - t') \int d^4x_1 \int d^4x_2 U(x_1)V(x_2)[\cdots].
$$

(30)

Moreover, we define the joint density $P_y(x,t) \equiv G(x,t|y)p_s(y)$ and following Ref. [31] introduce the dual-reversed current operator $\hat{j}_x^\dagger \equiv \mathbf{j}_s(x)/p_s(x) + \mathbf{D} p_s(x) \nabla x p_s^{-1}(x) = -\hat{j}_x (\mathbf{j}_s \rightarrow -\mathbf{j}_s)$. With these notations, using integration by parts, and by relabeling $x_1 \leftrightarrow x_2$ in one term, we rewrite Eq. (28) to obtain for the correlation, reproducing the main result of Refs. [30,31],

$$
\langle \mathbf{J}_t \rho_t \rangle_s - \langle \mathbf{J}_t \rangle_s \langle \rho_t \rangle_s = \hat{T}_{x_1y} \left[ \hat{j}_{x_1}^\dagger P_{x_2}(x_1,t') + \mathbf{j}_s(x_1)p_s^{-1}(x_1)P_{x_1}(x_2,t') + \mathbf{D} p_s(x_1) \nabla_{x_1} p_s(x_1)^{-1}P_{x_1}(x_2,t') \right] - \langle \mathbf{J}_t \rangle_s \langle \rho_t \rangle_s
$$

$$
= \hat{T}_{x_1y} \left[ \hat{j}_{x_1}^\dagger P_{x_2}(x_1,t') + \mathbf{j}_s^\dagger(x_2)P_{x_1}(x_2,t') - 2\mathbf{j}_s(x_1)p_s(x_2) \right],
$$

(31)

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

Instead of obtaining $\langle \rho_t^2 \rangle_s$ from the $\nu^2$ order in Eq. (26) we here consider a generalization to two densities, $\rho_t = \int_0^t V(x_2) \rho_t' = \int_0^t U(x_2 \rho_t \d \tau \rho_t' = \int_0^t U(x_2 \rho_t \d \tau \rho_t'$ is obtained equivalently and gives $\hat{L}(x,v,v') = \hat{L}(x) - ivV(x) - iv'U(x)$. The Fourier-transformed tilted generator in Eq. (21) with Fourier variables $\nu, \omega'$ corresponding to $\rho_t, \rho_t'$ is obtained equivalently and gives $\hat{L}(x,v,v') = \hat{L}(x) - ivV(x) - iv'U(x)$. The related term in the Dyson series (by an adaption of Eq. (26) including $\nu'U$) becomes $[\nu V(x_2) + \nu'U(x_2)]G(x_2,t_2 - t_1|x_1)[\nu V(x_1) + \nu'U(x_1)]p_s(x_1)$ (see also [34]). By comparison with the characteristic function in Eq. (22) including $\rho'_t$, one obtains the known result [9,34],

$$
\langle \rho_t^2 \rangle_s - \langle \rho_t \rangle_s \langle \rho_t \rangle_s = \hat{T}_{x_1y} [P_{x_2}(x_1,t') + P_{x_1}(x_2,t') - 2p_s(x_1)p_s(x_2)].
$$

(32)
For \( U = V \) this becomes the variance of \( \rho_t \) which can also be obtained from the order \( \nu^2 \) in Eqs. (22) and (26).

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

\[
\hat{L}(x, \omega, \omega') = \dot{L}(x) - i \omega^T \cdot \dot{L}^U(x) - i \omega'^T \cdot \dot{L}^V(x) - U(x)^2 \omega^T D \omega - V(x)^2 \omega'^T D \omega' - 2U(x)V(x)\omega^T D \omega' \\
\dot{L}^V(x) \equiv V(x)\dot{j}_x - D \nabla x V(x).
\]

(33)

The Dyson series (by adapting Eq. (26)) based on \( \hat{L}(x, \omega, \omega') \) for two currents \( J, J' \) reads

\[
\hat{P}_{J,J'}(\omega, \omega'|p_s) = 1 - \int d^d x_1 \int_0^t dt_1 \left[ i \omega^T \cdot \dot{L}^U(x_1) + i \omega'^T \cdot \dot{L}^V(x_1) + 2U(x_1)V(x_1)\omega^T D \omega' \right] p_s(x_1) \\
+ \int d^d x_1 \int d^d x_2 \int_0^t dt_2 \int_0^{t_2} dt_1 \left[ i \omega^T \cdot \dot{L}^U(x_2) + i \omega'^T \cdot \dot{L}^V(x_2) \right] G(x_2, t_2 - t_1 | x_1) \left[ i \omega^T \cdot \dot{L}^U(x_1) + i \omega'^T \cdot \dot{L}^V(x_1) \right] p_s(x_1) + O(\omega^2, \omega'^2).
\]

(34)

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

\[
\langle J_{t,n}J'_{t,m} \rangle_s = 2t D_{nm} \int d^d x_1 U(x_1) V(x_1) p_s(x_1) + \int_0^t dt' (t - t') \int d^d x_1 \int d^d x_2 \left[ \dot{L}^U_n(x_2) G(x_2, t'|x_1) \cdot \dot{L}^U_m(x_1) p_s(x_1) + \dot{L}^V_n(x_2) G(x_2, t'|x_1) \cdot \dot{L}^V_m(x_1) p_s(x_1) \right].
\]

(35)

We denote by \( \dot{=} \) equality up to gradient terms that vanish upon integration to write

\[
\dot{L}^U_n(x_2) G(x_2, t'|x_1) \cdot \dot{L}^V_m(x_1) p_s(x_1) \dot{=} U(x_2) \dot{j}_{x_2,n} G(x_2, t'|x_1) \times \\
[V(x_1) \dot{j}_s(x_1) p_s^{-1}(x_1) - p_s(x_1) D \nabla x_1 p_s^{-1}(x_1) - D \nabla x_1 V(x_1)]_{m} p_s(x_1) \\
\dot{=} U(x_2) V(x_1) \dot{j}_{x_2,n} \dot{j}_{x_1,m} p_s(x_1) + p_s(x_1) D \nabla x_1 p_s^{-1}(x_1)]_{m} G(x_2, t'|x_1) p_s(x_1) \\
= U(x_2) V(x_1) \dot{j}_{x_2,n} \dot{j}_{x_1,m} P_{x_1}(x_2, t).
\]

(36)

Inserting this into Eq. (35), and relabeling in one term \( x_1 \leftrightarrow x_2 \) we obtain for the \( nm \)-element of the current covariance matrix

\[
\langle J_{t,n}J'_{t,m} \rangle_s - \langle J_{t,n} \rangle_s \langle J'_{t,m} \rangle_s = 2t D_{nm} \int d^d x_1 U(x_1) V(x_1) p_s(x_1) \\
+ \dot{T}_{x_y} \left[ \dot{j}_{x_1,m} \dot{j}_{x_2,n} P_{x_1}(x_1, t') + \dot{j}_{x_2,n} \dot{j}_{x_1,m} P_{x_1}(x_2, t') \right].
\]

(37)

This reproduces and slightly generalizes the main result of Refs. [30, 31] where the diagonal elements \( (m = n) \) of the covariance matrix were derived. This result for
the current covariance matrix and Eq. (31) for the current-density correlation are the natural generalizations of the density-density covariance Eq. (32), as described in detail in references [30, 31], with the additional $2tD_{nm}$-term in Eq. (37) arising from the $(dW_\tau)^2$ contribution in $J_{t,n}J_{t,m}$ manifested in the term $-2U(x)V(x)\omega^T D \omega'$ in the tilted generator in Eq. (33). While the density-density covariance Eq. (32) only depends on integration over all paths from $x_1$ to $x_2$ (and vice versa) in time $t'$ via $P_{x_1}(x_2, t')$, the current-density correlation Eq. (31) instead involves $\hat{j}_{x_2} P_{x_2}(x_1, t')$ and $\hat{j}^\dagger_{x_1} P_{x_1}(x_2, t')$ which describe currents at the final- and initial-points, respectively [31]. This notion is further extended in the result Eq. (37) where $\hat{j}_{x_2} n_{x_1} \hat{j}^\dagger_{x_1} m P_{x_1}(x_2, t')$ corresponds to products of components of displacements along individual trajectories from $x_1$ to $x_2$ [30].

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. These two approaches illustrate how one can freely choose between Itô and functional calculus to derive results on dynamical functionals. In particular, both approaches are accessible without further technical mathematical concepts such as the Cameron-Martin-Girsanov theorem that is often used in the study of tilted generators. Our methodological advance thus provides a flexible repertoire of easily accessible methods that will hopefully prove useful in future studies of related problems.

The derivation of the moments and correlations based on the tilted generator reproduces results with important implications for stochastic thermodynamics and large deviation theory, in particular for the physical and mathematical role of coarse graining [30, 31], and thereby displays how the tilted generator yields results on the statistics of dynamical functionals, even beyond the large deviation limit.

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Data availability statement

No new data were created or analysed in this study.

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