Check for
updates

Manifestations of Projection-Induced Memory: General Theory and the Tilted Single File

Alessio Lapolla and Aljaž Godec*

Mathematical Biophysics Group, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Over the years the field of non-Markovian stochastic processes and anomalous diffusion evolved from a specialized topic to mainstream theory, which transgressed the realms of physics to chemistry, biology and ecology. Numerous phenomenological approaches emerged, which can more or less successfully reproduce or account for experimental observations in condensed matter, biological and/or single-particle systems. However, as far as their predictions are concerned these approaches are not unique, often build on conceptually orthogonal ideas, and are typically employed on an *ad-hoc* basis. It therefore seems timely and desirable to establish a systematic, mathematically unifying and clean approach starting from more fine-grained principles. Here we analyze projection-induced ergodic non-Markovian dynamics, both reversible as well as irreversible, using spectral theory. We investigate dynamical correlations between histories of projected and latent observables that give rise to memory in projected dynamics, and rigorously establish conditions under which projected dynamics is Markovian or renewal. A systematic metric is proposed for quantifying the degree of non-Markovianity. As a simple, illustrative but non-trivial example we study single file diffusion in a tilted box, which, for the first time, we solve exactly using the coordinate Bethe ansatz. Our results provide a solid foundation for a deeper and more systematic analysis of projection-induced non-Markovian dynamics and anomalous diffusion.

Keywords: Fokker-Planck equation, spectral theory, projection operator method, occupation time, single file diffusion, Bethe ansatz, free energy landscape

1. INTRODUCTION

Over the past decades the field of anomalous diffusion and non-Markovian dynamics grew to a mainstream physical topic [1–10] backed up by a surge of experimental observations [11–16] (the list of works is anything but exhaustive). From a theoretical point of view the description of anomalous and non-Markovian phenomena is not universal [1] and can be roughly (and judiciously) classified according to the underlying phenomenology: (i) renewal continuous-time random walk and fractional Fokker-Planck approaches [1–3, 17, 18], (ii) diffusion in disordered media [19–27], (iii) generalized Langevin equation descriptions [28–36], (iv) spatially heterogeneous diffusion [37–43], and more recently also (v) the so-called diffusing diffusivity models [44–50].

From a more general first-principles perspective non-Markovian dynamics in physical systems are always a result of the projection of nominally deterministic and/or Markovian high-dimensional dynamics to a lower-dimensional subspace [51–60]. The projection in general induces a

dependence of the dynamics on the initial conditions of the latent degrees of freedom, i.e., those being integrated out, thereby leading to memory [51, 54–56] and possibly (depending on the system) also to anomalous diffusion [61–68].

Hallmarks of broken Markovianity are the non-validity of the Chapman–Kolmogorov equation, and, on the level of individual trajectories, correlations between histories of projected observables and latent degrees of freedom [67]. The advantage of a first principles approach is that it allows for a deeper understanding and complete control over the origin and nature of memory effects. It might, however, be difficult to integrate out exactly degrees of freedom in a given microscopic model, and in practice this seems to be only possible for simple models, e.g., harmonic systems (e.g., [69]), comb-models (e.g., [70–72]) or simple obstruction models [61–67], to name but a few.

Here, instead of deriving effective evolution operators for projected dynamics [51, 54–56] we use a spectral-theoretic approach and focus on the consequences of the projection directly on the level of probability density functions of projected variables—both in a general setting as well as by means of a simplistic yet non-trivial model of single file diffusion in a tilted box. Using spectral theory we first present a rigorous and quite general analysis of the problem and establish conditions, under which the projection in fact leads to Markovian or renewal-type dynamics. We then apply these general results to the analysis of tagged particle diffusion in a single file confined in a tilted box. We obtain an exact solution of the full many-body and projected tagged particle propagators using the coordinate Bethe ansatz, and provide exact results for tagged particle local time statistics and correlations between tagged particle histories. Finally, to asses the degree of non-Markovianity induced by the projection, we compute the Kullback–Leibler divergence between the exact tagged particle propagator and the propagator of Markovian diffusion in the respective free energy landscape, i.e., in the so-called free energy landscape perspective. Our results provide a deeper understanding of projection-induced memory and anomalous diffusion and highlight important pitfalls in applications of free energy landscape-ideas in absence of a time-scale separation.

2. THEORY

2.1. Notation and Mathematical Preliminaries

Although all presented result hold identically for discrete-state jump dynamics governed by a Markovian master equation we will here throughout be interested in projections of strongly Markovian diffusion in continuous time and in a continuous domain $\Omega \in \mathbb{R}^d$ in a vector field $\mathbf{F}(\mathbf{x}) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ (not necessarily a potential field), which is either nominally confining (in this case Ω is open) or is accompanied by corresponding reflecting boundary conditions at $\partial\Omega$ (in this case Ω is closed) thus guaranteeing the existence of an invariant measure and hence ergodicity. The dynamics are governed by the (forward) Fokker-Planck operator $\hat{\mathcal{L}} : V \rightarrow V$ or its adjoint (or backward) operator $\hat{\mathcal{L}}^{\dagger} : W \rightarrow W$, where V is a complete normed linear

vector space with elements $f \in C^2(\mathbb{R}^d)$, and W is the space dual to V. In particular,

$$\hat{\mathcal{L}} = \nabla \cdot \mathbf{D}\nabla - \nabla \cdot \mathbf{F}(\mathbf{x}), \qquad \hat{\mathcal{L}}^{\dagger} = \nabla \cdot \mathbf{D}\nabla + \mathbf{F}(\mathbf{x}) \cdot \nabla, \quad (1)$$

where $\mathbf{D}$ is the symmetric positive-definite diffusion matrix. $\hat{\mathcal{L}}$ propagates probability measures $\mu_t(\mathbf{x})$ in time, which will throughout be assumed to posses well-behaved probability density functions $P(\mathbf{x}, t)$, i.e., $d\mu_t(\mathbf{x}) = P(\mathbf{x}, t)d\mathbf{x}$ [thereby posing some restrictions on $\mathbf{F}(\mathbf{x})$]. On the level of individual trajectories Equation (1) corresponds to the Itô equation $d\mathbf{x}_t = \mathbf{F}(\mathbf{x}_t)dt + \boldsymbol{\sigma}\,d\mathbf{W}_t$ with $\mathbf{W}_t$ being a d-dimensional vector of independent Wiener processes whose increments have a Gaussian distribution with zero mean and variance dt, i.e., $\langle dW_{t,i}dW_{t',j}\rangle = \delta_{ij}\delta(t - t')dt$, and where $\boldsymbol{\sigma}$ is a $d \times d$ symmetric noise matrix such that $\mathbf{D} = 2\boldsymbol{\sigma}\boldsymbol{\sigma}^T$. Moreover, we assume that $\mathbf{F}(\mathbf{x})$ admits the following decomposition into a potential (irrotational) field $-\mathbf{D}\nabla\varphi(\mathbf{x})$ and a non-conservative component $\boldsymbol{\vartheta}(\mathbf{x})$, $\mathbf{F}(\mathbf{x}) = -\mathbf{D}\nabla\varphi(\mathbf{x}) + \boldsymbol{\vartheta}(\mathbf{x})$ with the two fields being mutually orthogonal $\nabla\varphi(\mathbf{x}) \cdot \boldsymbol{\vartheta}(\mathbf{x}) = 0$ [73]. By insertion into Equation (1) one can now easily check that $\hat{\mathcal{L}}e^{-\varphi(\mathbf{x})} = 0$, such that the stationary solution of the Fokker-Planck equation (also referred to as the steady state [74, 75], which is the terminology we adopt here) by construction does not depend on the non-conservative part $\boldsymbol{\vartheta}(\mathbf{x})$. Before proceeding we first establish the decomposition of the drift field $\mathbf{F}(\mathbf{x})$ of the full dynamics, which with the knowledge of $\varphi(\mathbf{x})$ can be shown to have the form

$$\mathbf{F}(\mathbf{x}) = -\mathbf{D}\nabla\varphi(\mathbf{x}) + e^{\varphi(\mathbf{x})}\mathbf{j}_{ss}(\mathbf{x}), \qquad (2)$$

$\mathbf{j}_{ss}(\mathbf{x})$ denoting the steady-state probability current and $\boldsymbol{\vartheta}(\mathbf{x}) \equiv e^{\varphi(\mathbf{x})}\mathbf{j}_{ss}(\mathbf{x})$ being incompressible. The proof follows straightforwardly. We take $\boldsymbol{\vartheta}(\mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{D}\nabla\varphi(\mathbf{x})$ and use $\varphi(\mathbf{x})$ to determine the steady-state current $\mathbf{j}_{ss}(\mathbf{x}) = (\boldsymbol{\vartheta}(\mathbf{x}) - \mathbf{D}\nabla\varphi(\mathbf{x}))e^{-\varphi(\mathbf{x})} + \mathbf{D}\nabla e^{-\varphi(\mathbf{x})}$, such that immediately $\boldsymbol{\vartheta}(\mathbf{x}) = e^{\varphi(\mathbf{x})}\mathbf{j}_{ss}(\mathbf{x})$ and in turn follows $\mathbf{F}(\mathbf{x})$ in Equation (2). To check for incompressibility we note that $\mathbf{j}_{ss}(\mathbf{x})$ is by definition divergence free and so $\nabla \cdot \boldsymbol{\vartheta}(\mathbf{x}) = e^{\varphi(\mathbf{x})}(\mathbf{j}_{ss}(\mathbf{x}) \cdot \nabla\varphi(\mathbf{x})) \equiv \boldsymbol{\vartheta}(\mathbf{x}) \cdot \nabla\varphi(\mathbf{x}) = 0$, i.e., $e^{\varphi(\mathbf{x})}\mathbf{j}_{ss}(\mathbf{x})$ is divergence-free, as claimed.

We define the forward and backward propagators by $\hat{U}(t) = e^{\hat{\mathcal{L}}t}$ and $\hat{U}^{\dagger}(t) = e^{\hat{\mathcal{L}}^{\dagger}t}$ such that $\hat{\mathcal{L}}$ and $\hat{\mathcal{L}}^{\dagger}$ are generators of a semi-group $\hat{U}(t + t') = \hat{U}(t)\hat{U}(t')$ and $\hat{U}^{\dagger}(t + t') = \hat{U}^{\dagger}(t)\hat{U}^{\dagger}(t')$, respectively. $\hat{\mathcal{L}}$ propagates probability measures $\mu_t(\mathbf{x})$ in time, whereas $\hat{\mathcal{L}}^{\dagger}$ propagates observables $\mathcal{A}(\mathbf{x}_t)$ in time, which is best seen from the definition of the expectation

$$\langle \mathcal{A}(\mathbf{x}_t)\rangle \equiv \int \mathcal{A}(\mathbf{x})d\mu_t(\mathbf{x}) = \int \mathcal{A}(\mathbf{x})e^{\hat{\mathcal{L}}t}P(\mathbf{x}, 0)d\mathbf{x} =$$
$$\int P(\mathbf{x}, 0)e^{\hat{\mathcal{L}}^{\dagger}t}\mathcal{A}(\mathbf{x})d\mathbf{x} \equiv \int d\mu_0(\mathbf{x}_0)\langle \mathcal{A}(\mathbf{x}_0, t)\rangle, \qquad (3)$$

where $\langle \mathcal{A}(\mathbf{x}_0, t)\rangle$ was defined to give a correct behavior after averaging over the realizations of the Itô process but before averaging over the initial conditions $P(\mathbf{x}, 0)$ for the forward in time process (or end-point conditions for the adjoint, backward

in time process). The propagation of measures by $\hat{\mathcal{L}}$ corresponds to the "Schrödinger" picture of quantum mechanics, whereas the propagation of observables resembles the "Heisenberg" picture.

For convenience we introduce the bra-ket notation with the "ket" $|f\rangle$ representing a vector in V (or W, respectively) written in position basis as $f(\mathbf{x}) \equiv \langle \mathbf{x}|f\rangle$, and the "bra" $\langle g|$ as the integral $\int d\mathbf{x}g^{\dagger}$. The scalar product is defined as $\langle g|f\rangle = \int d\mathbf{x}g^{\dagger}(\mathbf{x})f(\mathbf{x})$. Therefore we have, in operator notation, the following evolution equation for the conditional probability density function starting from an initial condition $|p_0\rangle$: $|p_t\rangle = e^{\hat{\mathcal{L}}t}|p_0\rangle$. Since the process is ergodic we have $\lim_{t\to\infty} e^{\hat{\mathcal{L}}t}|p_0\rangle = |\mathrm{ss}\rangle$, where we have defined the equilibrium or non-equilibrium steady state, $\hat{\mathcal{L}}|\mathrm{ss}\rangle = 0$ and $\langle \mathrm{ss}|\hat{\mathcal{L}}^{\dagger} = 0$, as a result of the duality. The steady state refers to a probability density function $\langle \mathbf{x}|\mathrm{ss}\rangle$ of the invarant measure, which might carry a time-independent non-vanishing probability current $\mathbf{j}_{\mathrm{ss}}(\mathbf{x})$. We also define the (typically non-normalizable) "flat" state $|-\rangle$, such that $\langle \mathbf{x}|-\rangle = 1$ and $\langle -|p_t\rangle = 1$. Hence, $\partial_t\langle -|p_t\rangle = 0$ and $\langle -|\hat{\mathcal{L}} = 0$ and $\hat{\mathcal{L}}^{\dagger}|-\rangle = 0$. We define the Green's function of the process as the conditional probability density function for a localized initial condition $\langle \mathbf{x}|p_0\rangle = \delta(\mathbf{x} - \mathbf{x}_0)$ as

$$G(\mathbf{x}, t|\mathbf{x}_0, 0) = \langle \mathbf{x}|\hat{U}(t)|\mathbf{x}_0\rangle \equiv \langle \mathbf{x}_0|\hat{U}^{\dagger}(t)|\mathbf{x}\rangle, \qquad (4)$$

such that the conditional probability density starting from a general initial condition $|p_0\rangle$ becomes $P(\mathbf{x}, t|p_0, 0) = \langle \mathbf{x}|\hat{U}(t)|p_0\rangle \equiv \int d\mathbf{x}_0 p_0(\mathbf{x}_0)G(\mathbf{x}, t|\mathbf{x}_0, 0)$. Moreover, as $\mathbf{F}(\mathbf{x})$ is assumed to be sufficiently confining (i.e., $\lim_{\mathbf{x}\to\infty} P(\mathbf{x}, t) = 0, \forall t$ sufficiently fast), such that $\hat{\mathcal{L}}$ corresponds to a coercive and densely defined operator on V (and $\hat{\mathcal{L}}^{\dagger}$ on W, respectively) [76–78]. Finally, $\hat{\mathcal{L}}$ is throughout assumed to be *normal*, i.e., $\hat{\mathcal{L}}^{\dagger}\hat{\mathcal{L}} - \hat{\mathcal{L}}\hat{\mathcal{L}}^{\dagger} = 0$ and thus henceforth $V = W$, where for reversible system (i.e., those obeying detailed balance) we have $\hat{\mathcal{L}}\hat{\mathcal{L}}^{\dagger} = \hat{\mathcal{L}}^{\dagger}\hat{\mathcal{L}} = 0$. Because any normal compact operator is diagonalizable [79], we can expand $\hat{\mathcal{L}}$ (and $\hat{\mathcal{L}}^{\dagger}$) in a complete bi-orthonormal set of left $\langle \psi_k^L|$ and right $|\psi_k^R\rangle$ ($\langle \psi_k^R|$ and $|\psi_k^L\rangle$, respectively) eigenstates

$$\hat{\mathcal{L}}|\psi_k^R\rangle = -\lambda_k|\psi_k^R\rangle, \qquad \hat{\mathcal{L}}^{\dagger}|\psi_k^L\rangle = -\alpha_k|\psi_k^L\rangle, \qquad (5)$$

with $\mathrm{Re}(\lambda_k) \geq 0$, and according to our definition of the scalar product we have

$$\langle \psi_k^L|\hat{\mathcal{L}}|\psi_k^R\rangle = -\lambda_k\langle \psi_k^L|\psi_k^R\rangle = \left(\langle \psi_k^R|\hat{\mathcal{L}}^{\dagger}|\psi_k^L\rangle\right)^{\dagger} = -\alpha_k^{\dagger}\langle \psi_k^R|\psi_k^L\rangle \qquad (6)$$

and hence the spectra of $\hat{\mathcal{L}}$ and $\hat{\mathcal{L}}^{\dagger}$ are complex conjugates, $\alpha_k = \lambda_k^{\dagger}$. Moreover, $\lambda_0 = 0$, $|\psi_0^R\rangle = |\mathrm{ss}\rangle$, $\langle \psi_0^L| = \langle -|$, and $\langle \psi_k^L|\psi_l^R\rangle = \delta_{kl}$. Finally, we also have the resolution of identity $\mathbf{1} = \sum_k |\psi_k^R\rangle\langle \psi_k^L|$ and the propagator $\hat{U}(t) = \sum_k |\psi_k^R\rangle\langle \psi_k^L|e^{-\lambda_k t}$. It follows that the spectral expansion of the Green's function reads

$$G(\mathbf{x}, t|\mathbf{x}_0, 0) = \sum_k \psi_k^R(\mathbf{x})\psi_k^{L\dagger}(\mathbf{x}_0)e^{-\lambda_k t} \equiv \sum_k \psi_k^L(\mathbf{x}_0)\psi_k^{R\dagger}(\mathbf{x})e^{-\lambda_k^{\dagger}t}, \qquad (7)$$

We now define, $\hat{\mathcal{P}}_{\mathbf{x}}(\mathbf{\Gamma}; \mathbf{q})$, a (potentially oblique) projection operator into a subspace of random variables – a mapping $\mathbf{q} = \mathbf{\Gamma}(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}^a$ to a subset of coordinates $\mathbf{q}$ lying in some orthogonal system in Euclidean space, $\mathbf{q} \in \Xi(\mathbb{R}^a) \subset \Omega(\mathbb{R}^d)$ with $a < d$. For example, the projection operator applied to some function $R(\mathbf{x}) \in V$ gives

$$\hat{\mathcal{P}}_{\mathbf{x}}(\mathbf{\Gamma}; \mathbf{q})R(\mathbf{x}) = \int_{\Omega} d\mathbf{x}\delta(\mathbf{\Gamma}(\mathbf{x}) - \mathbf{q})R(\mathbf{x}). \qquad (8)$$

The spectral expansion of $\hat{\mathcal{L}}$ (and $\hat{\mathcal{L}}^{\dagger}$) in the bi-orthogonal Hilbert space alongside the projection operator $\hat{\mathcal{P}}_{\mathbf{x}}(\mathbf{\Gamma}; \mathbf{q})$ will now allow us to define and analyze projection-induced non-Markovian dynamics.

2.2. General Results
2.2.1. Non-Markovian Dynamics and (Non)Existence of a Semigroup

Using the projection operator $\hat{\mathcal{P}}_{\mathbf{x}}(\mathbf{\Gamma}; \mathbf{q})$ defined in Equation (8) we can define the (in general) non-Markovian Green's function of the projected dynamics as the conditional probability density of projected dynamics starting from a localized initial condition $\mathbf{q}_0$

$$Q_{p_0}(\mathbf{q}, t|\mathbf{q}_0, 0) = \frac{Q_{p_0}(\mathbf{q}, t, \mathbf{q}_0, 0)_{p_0}}{Q_{p_0}^0(\mathbf{q}_0)}$$

$$\equiv \frac{\hat{\mathcal{P}}_{\mathbf{x}}(\mathbf{\Gamma}; \mathbf{q})\hat{\mathcal{P}}_{\mathbf{x}_0}(\mathbf{\Gamma}; \mathbf{q}_0)G(\mathbf{x}, t|\mathbf{x}_0, 0)p_0(\mathbf{x}_0)}{\hat{\mathcal{P}}_{\mathbf{x}_0}(\mathbf{\Gamma}; \mathbf{q}_0)p_0(\mathbf{x}_0)}, \qquad (9)$$

which demonstrates that the time evolution of projected dynamics starting from a fixed condition $\mathbf{q}_0$ depends on the initial preparation of the full system $p_0(\mathbf{x}_0)$ as denoted by the subscript. This is a first signature of the non-Markovian and non-stationary nature of projected dynamics and was noted upon also in [55]. Obviously, $\int_{\Xi} d\mathbf{q}Q_{p_0}(\mathbf{q}, t|\mathbf{q}_0, 0) = 1$ for any initial condition $\mathbf{q}_0$. We will refer to $\mathbf{q}$ as the projected degrees of freedom, whereas those integrated out will be called latent. For the sake of simplicity we will here mostly limit our discussion to a stationary preparation of the system, i.e., $p_0(\mathbf{x}_0) = p_{\mathrm{ss}}(\mathbf{x}_0) = \langle \mathbf{x}_0|\mathrm{ss}\rangle$. In order to avoid duplicating results we will explicitly carry out the calculation with the spectral expansion of $\hat{\mathcal{L}}$ but note that equivalent results are obtained using $\hat{\mathcal{L}}^{\dagger}$. Using the spectral expansion Equation (7) and introducing $\Psi_{kl}(\mathbf{q})$, the elements of an infinite-dimensional matrix

$$\Psi_{kl}(\mathbf{q}) = \langle \psi_k^L|\delta(\mathbf{\Gamma}(\mathbf{x}) - \mathbf{q})|\psi_l^R\rangle \qquad (10)$$

we find from Equation (9)

$$Q_{p_{\mathrm{ss}}}(\mathbf{q}, t|\mathbf{q}_0, 0) = \sum_k \Psi_{0k}(\mathbf{q})(\Psi_{k0}(\mathbf{q}_0)/\Psi_{00}(\mathbf{q}_0))e^{-\lambda_k t} \qquad (11)$$

with $\Psi_{00}(\mathbf{q}_0) = Q_{p_{\mathrm{ss}}}^0(\mathbf{q}_0)$. If one would to identify $\Psi_{0k}(\mathbf{q}) = \Psi_{0k}^R(\mathbf{q})$ and $\Psi_{00}(\mathbf{q}_0)^{-1}\Psi_{0k}(\mathbf{q}) = \Psi_{0k}^L(\mathbf{q})$, Equation (11) at first sight looks deceivingly similar to the Markovian Green's function in Equation (7). Moreover, a hallmark of Markovian dynamics is that it obeys the Chapman–Kolmogorov equation and indeed,

since $\langle \psi_k^L | \psi_l^R \rangle = \delta_{kl}$, we find from the spectral expansion Equation (7) directly for any $0 < t' < t$ that

$$
\begin{aligned}
\int_\Omega d\mathbf{x}' G(\mathbf{x}, t | \mathbf{x}', t') G(\mathbf{x}', t' | \mathbf{x}_0, 0) \\
= \sum_{k,l} \psi_k^R(\mathbf{x}) \langle \psi_k^L | \psi_l^R \rangle \psi_l^{L\dagger}(\mathbf{x}_0) e^{-\lambda_k(t-t') - \lambda_l t'} \\
\equiv G(\mathbf{x}, t | \mathbf{x}_0, 0). \quad (12)
\end{aligned}
$$

For non-Markovian dynamics with a stationary $p_0(\mathbf{x})$ we here prove the following

Proposition 2.2.1.1. *Let the full system be prepared in a steady state, $p_0(\mathbf{x}) = p_{ss}(\mathbf{x})$, and let non-Markovian Green's function be defined by Equation (9). We take $\Psi_{kl}(\mathbf{q})$ as defined in Equation (10) and define a scalar product with respect to a Lebesgue measure w as $\langle f | g \rangle_w \equiv \int d\mathbf{x} w(\mathbf{x}) f^\dagger(\mathbf{x}) g(\mathbf{x})$. Then the Green's function of the projected process will obey the Chapman–Kolmogorov equation if and only if $\langle \Psi_{l0} | \Psi_{k0} \rangle_{\Psi_{00}^{-1}} = 0, \forall k, l$.*

We need to prove if and under which conditions

$$
\int_\Xi d\mathbf{q}' Q_{p_{ss}}(\mathbf{q}, t | \mathbf{q}', t') Q_{p_{ss}}(\mathbf{q}', t' | \mathbf{q}_0, 0) \quad (13)
$$

can be equal to $Q_{p_{ss}}(\mathbf{q}, t | \mathbf{q}_0, 0)$. As this will generally not be the case this essentially means that the projected dynamics is in general non-Markovian. The proof is established by noticing that $\Psi_{kl}(\mathbf{q}') = \Psi_{lk}^\dagger(\mathbf{q}')$ such that $\langle \Psi_{l0} | \Psi_{k0} \rangle_{\Psi_{00}^{-1}} \equiv \int_\Xi d\mathbf{q}' \Psi_{00}(\mathbf{q}')^{-1} \Psi_{0l}(\mathbf{q}') \Psi_{k0}(\mathbf{q}') \, \Psi_{00}(\mathbf{q}')^{-1} d\mathbf{q}$. As a result Equation (13) can be written analogously to the first equality in Equation (12) as

$$
\sum_{k,l} \Psi_{0k}(\mathbf{q}) \langle \Psi_{l0} | \Psi_{k0} \rangle_{\Psi_{00}^{-1}} (\Psi_{0l}^\dagger(\mathbf{q}_0) / \Psi_{00}(\mathbf{q}_0)) e^{-\lambda_k(t-t') - \lambda_l t'}. \quad (14)
$$

But since the projection mixes all excited eigenstates with $k > 0$ (to a k-dependent extent) with the left and right ground states [see Equation (10)], the orthogonality between $\Psi_{00}(\mathbf{q})^{-1/2} \Psi_{0l}(\mathbf{q})$ and $\Psi_{00}(\mathbf{q})^{-1/2} \Psi_{k0}(\mathbf{q})$ is in general lost, and $\langle \Psi_{l0} | \Psi_{k0} \rangle_{\Psi_{00}^{-1}} \neq 0$ for $k \neq l$ as claimed above. The Chapman–Kolmogorov equation can hence be satisfied if and only if $\langle \Psi_{l0} | \Psi_{k0} \rangle_{\Psi_{00}^{-1}} = 0$ for all $k \neq l$.

The possibility that the Chapman–Kolmogorov equation remains valid for non-Markovian process has been demonstrated previously on the hand of specific models (see e.g., [80, 81]). Here we establish the necessary and sufficient conditions for this to be the case in a quite general setting. In turn, even if $\langle \Psi_{l0} | \Psi_{k0} \rangle_{\Psi_{00}^{-1}} = 0, \forall k \neq l$ that this does not guarantee that the projected process is actually Markovian. The computation of higher-order probability densities is necessary in order to check for Markovianity.

2.2.2. When Is the Projected Dynamics Markovian or Renewal?
A) Projected Dynamics is Markovian

A particularly useful aspect of the present spectral-theoretic approach is its ability to establish rigorous conditions for the emergence of (exactly) Markovian and (exactly) renewal-type dynamics from a microscopic, first principles point of view. Note that in this section we assume a general, non-stationary preparation of the system [i.e., $p_0(\mathbf{x}_0) \neq p_{ss}(\mathbf{x}_0)$]. By inspection of Equations (10) and (11) one can establish that:

Theorem 2.2.2.1. *The necessary and sufficient condition for the projected dynamics to be Markovian if is that the projection $\hat{\mathcal{P}}_\mathbf{x}(\mathbf{\Gamma}; \mathbf{q})$ (whatever its form) nominally projects into the nullspace of latent dynamics. In other words, the latent and projected dynamics remain decoupled and orthogonal for all times. This means that (i) there exists a bijective map $\mathbf{y} = f(\mathbf{x})$ to a decomposable coordinate system $\mathbf{y} = (\mathbf{q}, \mathbf{q}'')$, in which the forward generator decomposes to $\hat{\mathcal{L}} = \hat{\mathcal{L}}_p + \hat{\mathcal{L}}_l$, where $\hat{\mathcal{L}}_p$ only acts and depends on the projected degrees of freedom $\mathbf{q} \in \Xi(\mathbb{R}^a) \subset \Omega(\mathbb{R}^d)$ with $a < d$ and $\hat{\mathcal{L}}_l$ only acts and depends on the latent coordinates $\mathbf{q}'' \in \Xi^c(\mathbb{R}^d) \subset \Omega(\mathbb{R}^d)$ (with, $\Xi \cap \Xi'' = \emptyset, \Omega = \Xi \cup \Xi''$), (ii) the boundary conditions on $\partial \Xi$ and $\partial \Xi^c$ are decoupled, and (iii) the projection operator $\hat{\mathcal{P}}_\mathbf{y}(\cdot; \mathbf{q}) = \int d\mathbf{q}''$ onto the subset of coordinates $\mathbf{q} \in \Xi(\mathbb{R}^a) \subset \Omega$ corresponds to an integral over the subset of latent coordinates $\mathbf{q}'' \in \Xi^c(\mathbb{R}^{d-a}) \subset \Omega$, which does not mix projected and latent degrees of freedom, or alternatively $\hat{\mathcal{L}}_l p_0(\mathbf{q}_0, \mathbf{q}_0'') = 0$.*

The statement of the theorem is intuitive and has most likely already been presented elsewhere in the existing literature, although we were not able to find it in the present form. The proof is rather straightforward and follows from the fact that if (and only if) the projected dynamics is Markovian it must be governed as well by a formal (Markovian) Fokker-Planck generator $\hat{\mathcal{L}}_p$ as in Equation (1), in which the projected and latent degrees of freedom are separable $\hat{\mathcal{L}} = \hat{\mathcal{L}}_p + \hat{\mathcal{L}}_l$, and that the full Hilbert space is a direct sum of Hilbert spaces of the $V = V_p \oplus V_l$, that is $\hat{\mathcal{L}}: V \to V, \hat{\mathcal{L}}_p: V_p \to V_p$ and $\hat{\mathcal{L}}_l: V_l \to V_l$ and $V_p \cap V_l = \emptyset$. This also requires that there is no boundary condition coupling vectors from V_p and V_l. In turn this implies assertion (i) above. If $\hat{\mathcal{P}}_\mathbf{y}(\cdot; \mathbf{q})$ is such that it does not mix eigenfunctions in V_p and V_l (i.e., it only involves vectors from V_p) then ecause of bi-orthonormality and the fact that $\langle -|\hat{\mathcal{L}} = 0$ the projected Green's function in full space $Q(\mathbf{q}, t | \mathbf{q}_0)$ for $\mathbf{q} \in \Xi(\mathbb{R}^a)$ will be identical to the full Green's function in the isolated domain $G(\mathbf{x}, t | \mathbf{x}_0)$ for $\mathbf{x} \in \Xi(\mathbb{R}^a)$ and the non-mixing condition is satisfied. The effect is the same if the latent degrees of freedom already start in a steady state, $\hat{\mathcal{L}}_l p_0(\mathbf{q}_0, \mathbf{q}_0'') = 0$. This establishes sufficiency. However, as soon as the projection mixes the two Hilbert spaces V_p and V_l, the generator of projected dynamics will pick up contributions from $\hat{\mathcal{L}}_l$ and will, upon integrating out the latent degrees of freedom, not be Markovian. This completes the proof.
B) Projected Dynamics is Renewal

We can also rigorously establish sufficient conditions for the projected dynamics to poses the renewal property. Namely, the physical notion of a waiting time or a random change of time-scale (see e.g., [2, 3]) can as well be attributed a microscopic origin. The idea of a random waiting time (or a random change of time scale) nominally implies a period of time and thereby the existence of some subdomain, during which and within the latent degrees evolve while the projected dynamics does not change. For this to be the case the latent degrees of freedom must be

perfectly orthogonal to the projected degrees of freedom, both in the two domains as well as on their boundaries (a prominent simple example is the so-called comb model [70–72]). Moreover, the projected degrees of freedom evolve only when the latent degrees of freedom reside in some subdomain $\Upsilon \subset \Xi^c(\mathbb{R}^{d-a})$. In turn, this means that the dynamics until a time t ideally partitions between projected and latent degrees of freedom, which are coupled solely by the fact that the total time spent in each must add to t, which effects the waiting time. In a comb-setting the motion along the backbone occurs only when the particle is in the center of the orthogonal plane. In the context of a low-dimensional projection of ergodic Markovian dynamics, we can in fact prove the following general theorem:

Theorem 2.2.2.2. *Let there exists a bijective map* $\mathbf{y} = f(\mathbf{x})$ *to a decomposable coordinate system* $\mathbf{y} = (\mathbf{q}, \mathbf{q}'')$ *as in A) with the projected* $\mathbf{q} \in \Xi(\mathbb{R}^a)$ *and latent degrees of freedom* $\mathbf{q}'' \in \Xi^c(\mathbb{R}^{d-a}) \equiv \Omega(\mathbb{R}^d) \setminus \Xi(\mathbb{R}^a)$. *Furthermore, let* $\Upsilon \subset \Xi^c(\mathbb{R}^{d-a})$ *and let* $\mathbb{1}_\Upsilon(\mathbf{q}'')$ *denote the indicator function of the region* Υ *(i.e.,* $\mathbb{1}_\Upsilon(\mathbf{q}'') = 1$ *if* $\mathbf{q}'' \in \Upsilon$ *and zero otherwise). Moreover, let the full system be prepared in an initial condition* $p_0(\mathbf{q}, \mathbf{q}'')$. *Then a sufficient condition for renewal-type dynamics is (i) that the forward generator in* $(\mathbf{q}, \mathbf{q}'')$ *decomposes* $\hat{\mathcal{L}} = \mathbb{1}_\Upsilon(\mathbf{q}'')\hat{\mathcal{L}}_p + \hat{\mathcal{L}}_l$, *and where* $\hat{\mathcal{L}}_p$ *only acts and depends on* $\mathbf{q}$ *and* $\hat{\mathcal{L}}_l$ *only acts and depends on* $\mathbf{q}''$, *and (ii) the boundary conditions do not cause a coupling of latent and projected degrees of freedom (as in the Markov case above).*

Theorem 2.2.2.2 and lemma 2.2.2.2.1 below appear to be new, and the proof can be established by an explicit construction of the exact evolution equation for the projected variables. Let $G_l(\mathbf{q}'', t | \mathbf{q}_0'')$ denote the Green's functions of the Markovian problem for the latent degrees of freedom, $G_l(\mathbf{q}'', t | \mathbf{q}_0'') = \langle \mathbf{q}'' | e^{\hat{\mathcal{L}}_l t} | \mathbf{q}_0'' \rangle = \sum_k \langle \mathbf{q}'' | \psi_k^{l,R} \rangle \langle \psi_k^{l,L} | \mathbf{q}_0'' \rangle e^{-\lambda_k^l t}$ and let $\tilde{g}(s) = \int_0^\infty e^{-st} g(t) dt$ denoted the Laplace transform of a function $g(t)$. The projection operator in this case corresponds to $\hat{\mathcal{P}}_{\mathbf{q}''}(\cdot; \mathbf{q}) = \int_{\Xi^c} d\mathbf{q}''$. We introduce the shorthand notation $\bar{p}_0(\mathbf{q}) = \int_{\Xi^c} d\mathbf{q}_0'' p_0(\mathbf{q}_0, \mathbf{q}_0'')$ and define the conditional initial probability density $p_0(\mathbf{q}_0'' | \mathbf{q}_0) = p_0(\mathbf{q}_0, \mathbf{q}_0'') / \bar{p}_0(\mathbf{q}_0)$. The Green's function of projected dynamics becomes $Q_{p_0}(\mathbf{q}, t | \mathbf{q}_0) = \int_{\Xi^c} d\mathbf{q}'' \int_{\Xi^c} d\mathbf{q}_0'' G(\mathbf{q}, \mathbf{q}'', t | \mathbf{q}_0, \mathbf{q}_0'') p_0(\mathbf{q}_0, \mathbf{q}_0'') / \bar{p}_0(\mathbf{q}_0)$. We then have the following

Lemma 2.2.2.2.1. *Under the specified assumptions* $Q(\mathbf{q}, t | \mathbf{q}_0)$ *exactly obeys the renewal-type non-Markovian Fokker-Planck equation*

$$\partial_t Q_{p_0}(\mathbf{q}, t | \mathbf{q}_0) = \int_0^t d\tau K_{p_0}(t - \tau) \hat{\mathcal{L}}_p Q_{p_0}(\mathbf{q}, \tau | \mathbf{q}_0), \quad (15)$$

with the memory kernel

$$K_{p_0}(t) = (\delta(t) + \partial_t) \int_\Upsilon d\mathbf{q}'' \int_{\Xi^c} d\mathbf{q}_0'' p_0(\mathbf{q}_0'' | \mathbf{q}_0) \langle \mathbf{q}'' | e^{\hat{\mathcal{L}}_l t} | \mathbf{q}_0'' \rangle$$

$$= \sum_k \left(\int_{\Xi^c} d\mathbf{q}_0'' \psi_k^{l,L\dagger}(\mathbf{q}_0'') p_0(\mathbf{q}_0'' | \mathbf{q}_0) \right)$$

$$\left(\int_\Upsilon d\mathbf{q}'' \psi_k^{l,R}(\mathbf{q}'') \right) (\delta(t) - \lambda_k^l e^{-\lambda_k^l t}) \quad (16)$$

that is independent of $\mathbf{q}$. *Moreover,* $Q(\mathbf{q}, t | \mathbf{q}_0) > 0$ *for all* $t > 0$ *and for all* $\mathbf{q}, \mathbf{q}_0 \in \Xi$.

To prove the lemma we Laplace transform equation ($t \to u$) $\partial_t G(\mathbf{q}, \mathbf{q}'', t | \mathbf{q}_0, \mathbf{q}_0'') = \hat{\mathcal{L}} G(\mathbf{q}, \mathbf{q}'', t | \mathbf{q}_0, \mathbf{q}_0'')$ and realize that the structure of $\hat{\mathcal{L}}$ implies that its solution with initial condition $\delta(\mathbf{q} - \mathbf{q}_0)\delta(\mathbf{q}'' - \mathbf{q}_0'')$ in Laplace space factorizes $\tilde{G}(\mathbf{q}, \mathbf{q}'', u | \mathbf{q}_0, \mathbf{q}_0'') = f_u(\mathbf{q} | \mathbf{q}_0) g_u(\mathbf{q}'' | \mathbf{q}_0'')$ with g_u and f_u to be determined. Note that $\int_\Xi d\mathbf{q} \int_{\Xi^c} d\mathbf{q}'' \tilde{G}(\mathbf{q}, \mathbf{q}'', u | \mathbf{q}_0, \mathbf{q}_0'') = \int_\Xi d\mathbf{q} f_u(\mathbf{q} | \mathbf{q}_0) \int_{\Xi^c} d\mathbf{q}'' g_u(\mathbf{q}'' | \mathbf{q}_0'') = u^{-1}$ and we can chose, without any loss of generality that $\int_\Xi d\mathbf{q} f_u(\mathbf{q} | \mathbf{q}_0) = 1$. Plugging in the factorized ansatz and rearranging leads to

$$g_u(\mathbf{q}'' | \mathbf{q}_0'') \left(u f_u(\mathbf{q} | \mathbf{q}_0) - \mathbb{1}_\Upsilon(\mathbf{q}'') \hat{\mathcal{L}}_p f_u(\mathbf{q} | \mathbf{q}_0) \right)$$

$$- f_u(\mathbf{q} | \mathbf{q}_0) \hat{\mathcal{L}}_l g_u(\mathbf{q}'' | \mathbf{q}_0'') - \delta(\mathbf{q} - \mathbf{q}_0)\delta(\mathbf{q}'' - \mathbf{q}_0'') = 0. \quad (17)$$

Noticing that $\int_\Xi d\mathbf{q} \hat{\mathcal{L}}_p f(\mathbf{q} | \mathbf{q}_0) = 0$ as a result of the divergence theorem (as we assumed that $\mathbf{F}(\mathbf{x})$ is strongly confining implying that the current vanishes at the boundaries) we obtain, upon integrating Equation (17) over $\mathbf{q}$

$$u g_u(\mathbf{q}'' | \mathbf{q}_0'') - \delta(\mathbf{q}'' - \mathbf{q}_0'') - \hat{\mathcal{L}}_l g_u(\mathbf{q}'' | \mathbf{q}_0'') = 0, \quad (18)$$

implying that $g_u(\mathbf{q}'' | \mathbf{q}_0'') = \tilde{G}_l(\mathbf{q}'', u | \mathbf{q}_0'')$. As $\tilde{G}_l(\mathbf{q}'', u | \mathbf{q}_0'')$ is the Laplace image of a Markovian Green's function we use $\int_{\Xi^c} d\mathbf{q}'' \tilde{G}_l(\mathbf{q}'', u | \mathbf{q}_0'') = u^{-1}$ in order to deduce that $\tilde{Q}_{p_0}(\mathbf{q}, u | \mathbf{q}_0) = f_u(\mathbf{q} | \mathbf{q}_0) / u$. The final step involves using the identified functions f_u and g_u in Equation (17), multiplying with $p_0(\mathbf{q}_0'' | \mathbf{q}_0)$, integrating over $\mathbf{q}''$ and $\mathbf{q}_0''$ while using the divergence theorem implying $\int_{\Xi^c} d\mathbf{q}'' \hat{\mathcal{L}}_l \tilde{G}_l(\mathbf{q}'', u | \mathbf{q}_0'') = 0$ (as before) to obtain

$$u \tilde{Q}_{p_0}(\mathbf{q}, u | \mathbf{q}_0) - \delta(\mathbf{q} - \mathbf{q}_0)$$

$$= \left(u \int_\Upsilon d\mathbf{q}'' \int_{\Xi^c} d\mathbf{q}_0'' \tilde{G}_l(\mathbf{q}'', u | \mathbf{q}_0'') p_0(\mathbf{q}_0'' | \mathbf{q}_0) \right) \hat{\mathcal{L}}_p \tilde{Q}_{p_0}(\mathbf{q}, u | \mathbf{q}_0). \quad (19)$$

Finally, since the Laplace transform of $\partial_t g(t) + \delta(t) g(0)$ corresponds to $u\tilde{g}(u)$, taking the inverse Laplace transform of Equation (19) finally leads to Equations (15) and (16) and completes the proof of the lemma, since now we can take $Q_{p_0}(\mathbf{q}, t | \mathbf{q}_0) > 0$ by definition because Equation (15) is an identity of Equation (1) integrated over $\mathbf{q}''$. Moreover, the rate of change of the Green's function $Q_{p_0}(\mathbf{q}, t | \mathbf{q}_0)$ in Equation (15) depends, at any instance t, position $\mathbf{q}$ and for any initial condition $\mathbf{q}_0$ only on the current position $\mathbf{q}$ and a waiting time (or random time-change) encoded in the memory kernel $K(t)$; $Q_{p_0}(\mathbf{q}, t | \mathbf{q}_0)$ is the Green's function of a renewal process. This completes the proof of sufficiency.

Furthermore, for the situation where the full system is prepared in a stationary state, i.e., $p_0(\mathbf{x}) = p_s(\mathbf{x})$, we have the following

Corollary 2.2.2.2.1. *Let the system and projection be defined as in Theorem 2.2.2.2. If the full system is prepared such that the latent degrees of freedom are in a stationary state* $p_0(\mathbf{q}_0, \mathbf{q}_0'')$, *such that*

$\hat{\mathcal{L}}_l p_0(\mathbf{q}_0''|\mathbf{q}_0) = 0, \forall \mathbf{q}_0 \in \Xi$ *and hence also* $\bar{p}_0(\mathbf{q}_0'') = \bar{p}_{ss}(\mathbf{q}_0'')$, *then* $p_0(\mathbf{q}_0''|\mathbf{q}_0) = \psi_0^{l,R}(\mathbf{q}_0'')$ *and consequently* $K_{p_0} = \delta(t) \int_\gamma d\mathbf{q}_0'' \bar{p}_{ss}(\mathbf{q}_0'')$, *and therefore the projected dynamics is Markovian. Moreover, if the system is prepared such that the latent degrees of freedom are not in a stationary state, i.e.,* $p_0(\mathbf{q}_0|\mathbf{q}_0'') \neq \bar{p}_{ss}(\mathbf{q}_0''), \forall \mathbf{q}_0$, *there exists a finite time* $t_M > 0$ *after which the dynamics will be arbitrarily close to being Markovian.*

The statement of this corollary is again intuitive. The proof of the first part follows from the bi-orthogonality of eigenfunctions of latent dynamics $\langle \psi_k^{l,R}|\psi_0^{l,R}\rangle = \delta_{k,0}$, rendering all terms in Equation (16) in Lemma 2.2.2.2.1 identically zero except for $k = 0$ with $\lambda_k^l = 0$. The second part is established by the fact that for times $t_M \gg 1/\lambda_1^l$, with $-\lambda_1^l$ being the largest (i.e., least negative) non-zero eigenvalue, all terms but the $k = 0$ term in Equation (16) in Lemma 2.2.2.2.1 become arbitrarily small.

Having established sufficiency, we now also comment on necessity of the conditions (i) and (ii) above for renewal dynamics. It is clear that the splitting of $\hat{\mathcal{L}}$ into $\hat{\mathcal{L}}_p$ and $\hat{\mathcal{L}}_l$, where $\hat{\mathcal{L}}_l$ does not act nor depend on projected variables, is also necessary condition for renewal. This can be established by contradiction as loosening these assumptions leads to dynamics that is not renewal. This can be understood intuitively, because it must hold that the latent degrees of freedom remain entirely decoupled from the projected ones (but not vice versa) and that the motion along both is mutually orthogonal. To illustrate this think of the paradigmatic comb model (see schematic in **Figure 1**) [70–72] and realize that renewal will be violated as soon as we tilt the side-branches for some angle from being orthogonal to the backbone.

However, since it is difficult to establish the most general class of admissible functions $h(\mathbf{q}'')$ used in $\hat{\mathcal{L}} = h(\mathbf{q}'')\hat{\mathcal{L}}_p + \hat{\mathcal{L}}_l$, we are not able to prove necessity. Based on the present
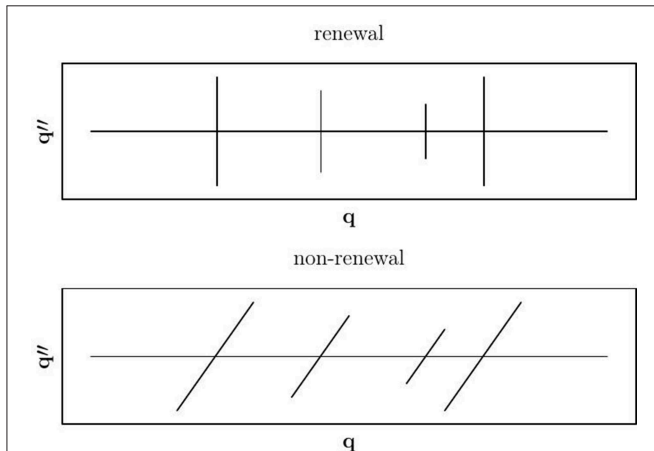

FIGURE 1 | Schematics of a generalized comb model. For the sake of clarity only a couple of side-branches are shown, whereas the model is to be understood in the sense of densely populated side-branches. (top) As long as the projected q and latent q'' degree of freedom remain orthogonal, the projected dynamics will be of renewal-type. However, as soon as this ceases to be the case the projected dynamics will not be renewal.

analysis it seems somewhat difficult to systematically relax the assumptions for projected dynamics to be renewal without assuming, in addition, some sort of spatial discretization. We therefore hypothesize that the sufficient conditions stated in Theorem 2.2.2.2, potentially with some additional assumptions on $h(\mathbf{q}'')$ are also necessary conditions. Notably, however, that microscopic derivations of non-Markovian master equations of the form given in Equation (15) often start in discretized space or *ad-hoc* introduce a random change in time scale (see e.g., [2, 17, 82]). We end this section with the following final

Remark 2.2.2.1. *An arbitrary projection* $\hat{\mathcal{P}}_\mathbf{x}(\mathbf{\Gamma}; \mathbf{q})$ *defined in Equation (8) will most likely lead to dynamics that is neither Markovian nor renewal.*

This follows from the strong assumptions required for Markovian and renewal dynamics, respectively. The properties of the corresponding general evolution operator will be described in a separate publication.

2.2.3. Markovian Approximation and the Degree of Non-Markovianity

In order to quantify the degree of non-Markovianity induced by the projection we propose to compare the full non-Markovian dynamics with projected dynamics evolving under a complete time-scale separation, i.e., under the assumption of all latent degrees of freedom being in the stationary state. To do so we proceed as follows. The projected coordinates $\mathbf{q}$ are now assumed to represent a subset of another d-dimensional orthogonal system in Euclidean space $\mathbf{q}' \in \mathbb{R}^d$, and we assume the map $\mathbf{q}'(\mathbf{x})$ is bijective. We denote the conditional probability density in this system by $G'(\mathbf{q}', t|\mathbf{q}_0', 0)$. The underlying physical idea is that an observer can only see the projected dynamics, which since it is non-Markovian stems from a projection but not necessarily onto Cartesian coordinates. Therefore, from a physical perspective not too much generality seems to be lost with this assumption.

As a concrete example one can consider the non-spherically symmetric Fokker-Planck process in a sphere, corresponding to the full Markovian parent system projected onto angular variables (either one or both). This way one first transforms from $\mathbf{x} \in \mathbb{R}^3$ to spherical coordinates $\mathbf{q}' = (r, \phi, \theta)$ and then, e.g., projects on the the lines $\mathbf{q} = \phi \in [0, 2\pi)$.

Since the transformation of the Fokker-Planck equation under a general change of coordinates is well-known [83] the task is actually simple. Under the complete map $\mathbf{q}' = \mathbf{\Gamma}(\mathbf{x})$ with $\mathbf{\Gamma}: \mathbb{R}^d \to \mathbb{R}^d$ the forward Fokker-Planck operator in Equation (1) transforms as $\hat{\mathcal{L}}' = \nabla_{\mathbf{q}'} \otimes \nabla_{\mathbf{q}'} : \tilde{D}(\mathbf{q}') - \nabla_{\mathbf{q}'} \cdot \tilde{\mathbf{F}}(\mathbf{q}')$, where $\otimes$ and $:$ denote, respectively, the tensor and double-dot product, and the transformed drift field and diffusion tensor can be written as

$$(\tilde{\mathbf{F}}(\mathbf{q}'))_k = \sum_{i=1}^d \frac{\partial q_k'}{\partial x_i} \mathbf{F}_i + \sum_{i,j=1}^d D_{ij} \frac{\partial^2 q_k}{\partial x_i \partial x_j},$$

$$(\tilde{D}(\mathbf{q}'))_{kl} = \sum_{i,j=1}^d D_{ij} \frac{\partial q_k'}{\partial x_i} \frac{\partial q_l'}{\partial x_j}. \qquad (20)$$

We note that unless the mapping is linear, the old diffusion matrix affects the new drift vector and the diffusion matrix picks up a spatial dependence. For an excellent account of the transformation properties in the more general case of a position dependent diffusion matrix [i.e., $\mathbf{D} \to \mathbf{D}(\mathbf{x})$] we refer the reader to [84]. We now want to marginalize over the remaining (i.e., non-projected) coordinates $\mathbf{q}'' \in \Omega \setminus \Xi$ but beforehand make the Markovian approximation $G'(\mathbf{q}', t | \mathbf{q}_0, 0) \approx Q_M(\mathbf{q}, t | \mathbf{q}_0) p_{ss}(\mathbf{q}'')$. Then we have $\hat{\mathcal{L}}' G'(\mathbf{q}', t | \mathbf{q}_0, 0) \approx p_{ss}(\mathbf{q}'') \hat{\mathcal{L}}' Q_M(\mathbf{q}, t | \mathbf{q}_0)$, implying that the operator $\hat{\mathcal{L}}'$ approximately splits into one part operating on the projected coordinates alone, $\hat{\mathcal{L}}'_M$, and one operating only on the latent stationary coordinates, $\hat{\mathcal{L}}''$, for which $\hat{\mathcal{L}}'' p_{ss}(\mathbf{q}'') = 0$. The physical idea behind the Markovian approximation is that the latent degrees of freedom relax infinitely fast compared to the projected ones. Therefore, we can straightforwardly average the Fokker-Planck operator over the stationary latent coordinates $\mathbf{q}''$, $\langle \hat{\mathcal{L}}'_M \rangle_{\mathbf{q}''}$, where we have defined the latent averaging operation $\langle \cdot \rangle_{\mathbf{q}''} \equiv \int d\mathbf{q}'' p_{ss}(\mathbf{q}'') \cdot$. Note that the remaining dependence of $\hat{\mathcal{L}}'$ on the latent stationary coordinates $\mathbf{q}''$ is only due to $\tilde{\mathbf{F}}(\mathbf{q}')$ and $\tilde{D}(\mathbf{q}')$. The averaged drift field and diffusion matrix now become

$$\langle \tilde{\mathbf{F}}(\mathbf{q}) \rangle_k = \sum_{i=1}^{d} \left\langle \frac{\partial q_k'}{\partial x_i} \mathbf{F}_i \right\rangle_{\mathbf{q}''} + \sum_{i,j=1}^{d} D_{ij} \left\langle \frac{\partial^2 q_k}{\partial x_i \partial x_j} \right\rangle_{\mathbf{q}''},$$

$$\langle \tilde{D}(\mathbf{q}) \rangle_{kl} = \sum_{i,j=1}^{d} D_{ij} \left\langle \frac{\partial q_k'}{\partial x_i} \frac{\partial q_l'}{\partial x_j} \right\rangle_{\mathbf{q}''}. \quad (21)$$

We can further decompose the effective drift field into a conservative and a non-conservative part

$$\left\langle \frac{\partial q_k'}{\partial x_i} \mathbf{F}_i \right\rangle_{\mathbf{q}''} = -\left\langle \frac{\partial q_k'}{\partial x_i} (\mathbf{D} \nabla \varphi)_i \right\rangle_{\mathbf{q}''} + \left\langle e^{\varphi} \frac{\partial q_k'}{\partial x_i} (\mathbf{j}_{ss})_i \right\rangle_{\mathbf{q}''}, \quad (22)$$

which establishes the Markovian approximation also for a broad class of irreversible systems. The approximate effective Fokker-Planck operator for the projected dynamics in turn reads

$$\langle \hat{\mathcal{L}}' \rangle_{\mathbf{q}''} = \nabla_{\mathbf{q}} \otimes \nabla_{\mathbf{q}} : \langle \tilde{D}(\mathbf{q}) \rangle_{\mathbf{q}''} - \nabla_{\mathbf{q}} \cdot \langle \tilde{\mathbf{F}}(\mathbf{q}) \rangle_{\mathbf{q}''}. \quad (23)$$

By design the kernel of $\langle \hat{\mathcal{L}}' \rangle_{\mathbf{q}''}$ is equal to $p_{ss}(\mathbf{q}) \equiv \hat{\mathcal{P}}_{\mathbf{x}}(\Gamma; \mathbf{q}) p_{ss}(\mathbf{x})$, hence $\langle \hat{\mathcal{L}}' \rangle_{\mathbf{q}''}$ governs the relaxation toward the steady-state density (not necessarily equilibrium) evolving from some initial state $\mathbf{q}_0$ in the Markovian approximation with the corresponding Green's function $Q_M(\mathbf{q}, t | \mathbf{q}_0, 0) \equiv \langle \mathbf{q} | e^{\langle \hat{\mathcal{L}}' \rangle_{\mathbf{q}''} t} | \mathbf{q}_0 \rangle$.

In order to quantify the departure of the exact dynamics from the corresponding Markovian behavior we propose to evaluate the Kullback–Leibler divergence between the Green's functions of the exact and Markovian propagator as a function of time

$$\mathcal{D}_t(Q || Q_M) = \int_{\Xi} d\mathbf{q} Q(\mathbf{q}, t | \mathbf{q}_0, 0) \ln \left(\frac{Q(\mathbf{q}, t | \mathbf{q}_0, 0)}{Q_M(\mathbf{q}, t | \mathbf{q}_0, 0)} \right). \quad (24)$$

By definition $\mathcal{D}_t(Q || Q_M) \geq 0$ and since the non-Markovian behavior of the exact projected dynamics is transient with a lifetime λ_1^{-1}, we have that $\lim_{t \to \infty} \mathcal{D}_t(Q || Q_M) = 0$. Our choice

of quantifying the departure of the exact dynamics from the corresponding Markovian behavior is not unique. The Kullback–Leibler divergence introduced here can hence be used to quantify how fast the correlation of the latent degrees of freedom with the projected degrees of freedom dies out. Notably, in a related manner the Kullback–Leibler divergence was also used in the context of stochastic thermodynamics in order to disprove the hypothesis about the monotonicity of the entropy production as a general time evolution principle [85].

2.2.4. Functionals of Projected Dynamics

In order to gain deeper insight into the origin and manifestation of non-Markovian behavior it is instructive to focus on the statistics of time-average observables, that is functionals of projected dynamics. As in the previous sections we assume that the full system was prepared in a (potentially non-equilibrium current-carrying) steady state. To that end we have, using Feynman-Kac theory, recently proven a theorem connecting any bounded additive functional $\Phi_t[\mathbf{q}(\tau)] = t^{-1} \int_0^t Z(\mathbf{q}(\tau)) d\tau$ (with a function $Z : \Xi(\mathbb{R}^a) \to \mathbb{R}$ locally strictly bounded in Ξ) of projected dynamics $\mathbf{q}(\tau)$ of a parent Markovian diffusion $\mathbf{x}(t)$ to the eigenspectrum of the Markov generator of the full dynamics $\hat{\mathcal{L}}$ or $\hat{\mathcal{L}}^\dagger$ [67]. The central quantity of the theory is $\theta_t(\mathbf{s})$, the so-called local time fraction spent by a trajectory $\mathbf{q}(\tau)$ in a infinitesimal volume element $d\mathbf{s}$ centered at $\mathbf{s}$ up until a time t enabling

$$\theta_t(\mathbf{s}) = t^{-1} \int_0^t d\tau \mathbb{1}_{\mathbf{s}}(\mathbf{q}(\tau)) \quad \to \quad \Phi_t[\mathbf{q}(\tau)] = \int_{\Xi} d\mathbf{s} Z(\mathbf{s}) \theta_t(\mathbf{s}), \quad (25)$$

where the indicator function $\mathbb{1}_{\mathbf{s}}(\mathbf{q}) = 1$ if $\mathbf{q} = \mathbf{s}$ and zero otherwise. We are here interested in the fluctuations of $\theta_t(\mathbf{s})$ and correlation functions between the local time fraction of a projected observable $\mathbf{q}(t)$ at a point $\mathbf{s}$ and $\theta''(\mathbf{s}')$, the local time some latent (hidden) observable $\mathbf{q}''(t)$ a the point $\mathbf{s}'$:

$$\sigma_t^2(\mathbf{s}) = \langle \theta_t^2(\mathbf{s}) \rangle - \langle \theta_t(\mathbf{s}) \rangle^2, \quad \mathcal{C}_t(\mathbf{s}; \mathbf{s}')$$
$$= \langle \theta_t(\mathbf{s}) \theta_t''(\mathbf{s}') \rangle - \langle \theta_t(\mathbf{s}) \rangle \langle \theta_t''(\mathbf{s}') \rangle, \quad (26)$$

where $\langle \cdot \rangle$ now denotes the average over all forward paths starting from the steady state $| \mathbf{q}_0 \rangle = | ss \rangle$ (and ending anywhere, i.e., $\langle \mathbf{q} | = \langle - |$), or, using the backward approach, all paths starting in the flat state $| \mathbf{q} \rangle = | - \rangle$ and propagating backward in time toward the steady state $\langle \mathbf{q}_0 | = \langle ss |$. We note that any correlation function of a general additive bounded functional $\Phi_t^i[\mathbf{q}(\tau)]$ of the form $\langle \Phi_t^i[\mathbf{q}(\tau)] \Phi_t^j[\mathbf{q}''(\tau)] \rangle$ (as well as the second moment of $\Phi_t^i[\mathbf{q}(\tau)]$) follows directly from the local time fraction, namely, $\langle \Phi_t^i[\mathbf{q}(\tau)] \Phi_t^j[\mathbf{q}''(\tau)] \rangle = \int_{\Xi} \int_{\Xi} d\mathbf{s} d\mathbf{s}' Z_i(\mathbf{s}) Z_j(\mathbf{s}') \langle \theta_t(\mathbf{s}) \theta_t''(\mathbf{s}') \rangle$. For details of the theory and corresponding proofs please see [67], here we will simply state the main result:

Theorem 2.2.4.1. *Let the Green's function of the full parent dynamics $\mathbf{x}(t)$ be given by Equation (7) and the local time fraction $\theta_t(\mathbf{s})$ by Equation (25), then the variance and correlation function*

defined in Equation (26) is given exactly as

$$\sigma_t^2(\mathbf{s}) = 2\sum_{k>0} \frac{\langle -|\mathbb{1}_{\mathbf{s}}|\psi_k^R\rangle\langle\psi_k^L|\mathbb{1}_{\mathbf{s}}|ss\rangle}{\lambda_k t}\left(1 - \frac{1-e^{-\lambda_k t}}{\lambda_k t}\right)$$

$$\mathcal{C}_t(\mathbf{s};\mathbf{s}') = \sum_{k>0} \frac{\langle -|\mathbb{1}_{\mathbf{s}}|\psi_k^R\rangle\langle\psi_k^L|\mathbb{1}_{\mathbf{s}'}''|ss\rangle + \langle -|\mathbb{1}_{\mathbf{s}'}''|\psi_k^R\rangle\langle\psi_k^L|\mathbb{1}_{\mathbf{s}}|ss\rangle}{\lambda_k t}$$

$$\left(1 - \frac{1-e^{-\lambda_k t}}{\lambda_k t}\right), \tag{27}$$

and analogous equations are obtained using the backward approach [67].

The usefulness of Equation (27) can be understood as follows. By varying $\mathbf{s}$ and $\mathbf{s}'$ one can establish *directly* the regions in space responsible for the build-up (and subsequent decay) of memory in projected dynamics and simultaneously monitor the fluctuations of the time spent of a projected trajectory in said regions. Note that because the full process is assumed to be ergodic, the statistics of $\theta_t(\mathbf{s})$ will be asymptotically Gaussian obeying the large deviation principle. This concludes our general results. In the following section we apply the theoretical framework to the analysis of projected dynamics in a strongly-correlated stochastic many-body system, namely to tagged particle dynamics in a single file confined to a tilted box.

3. SINGLE FILE DIFFUSION IN A TILTED BOX

We now apply the theory developed in the previous section (here we use the backward approach) to the paradigmatic single file diffusion in a unit interval but here with a twist, namely, the diffusing particles experience a constant force. In particular, the full state-space is spanned by the positions of all N-particles defining the state vector $\mathbf{x}_0 = (x_{0,1},\ldots,x_{0,N})^T \in [0,1]^N$ and diffusion coefficients of all particles are assumed to be equal and the thermal (white) fluctuations due to the bath are assumed to be independent, i.e., $\mathbf{D} = D\mathbb{1}$. In addition to being confined in a unit interval, all particles experience the same constant force $\mathbf{F}(\mathbf{x}_0) = -\beta DF$ with $\beta = (k_BT)^{-1}$ is the inverse thermal energy. The evolution of the Green's function is governed by the Fokker-Planck equation Equation (1) equipped with the external and internal (i.e., non-crossing) reflecting boundary conditions for the backward generator $\hat{\mathcal{L}}^\dagger = \sum_{i=1}^N D(\partial_{x_{0,i}}^2 - \beta F\partial_{x_{0,i}})$:

$$\partial_{x_{0,1}} G(\mathbf{x},t|\mathbf{x}_0)|_{x_{0,1}=0} = \partial_{x_{0,N}} G(\mathbf{x},t|\mathbf{x}_0)|_{x_{0,N}=1} = 0,$$

$$\lim_{x_{0,i}\to x_{0,j}}(\partial_{x_{0,i+1}} - \partial_{x_{0,i}})G(\mathbf{x},t|\mathbf{x}_0) = 0, \tag{28}$$

where we adopted the notation in Equation (7). The boundary conditions in Equation (28) restrict the domain to a hypercone $\mathbf{x}_0 \in \Xi$ such that $x_{0,i} \leq x_{0,i+1}$ for $i = 1,\ldots,N-1$. The dynamics is reversible, hence the steady state current vanishes and all eigenvalues and eigenfunctions are real. Moreover, for systems obeying detailed balance $\varphi(\mathbf{x})$ corresponds to the density of the Boltzmann-Gibbs measure and it is known that $|\psi_k^L\rangle \equiv e^{-\varphi(\mathbf{x})}|\psi_k^R\rangle$. The single file backward generator already has a

separated form $\hat{\mathcal{L}}^\dagger = \sum_{i=1}^N \mathcal{L}_i^\dagger$ and the coupling between particles enters solely through the non-crossing boundary condition Equation (28) and is hence Bethe-integrable [86]. However, because the projected and latent degrees of freedom are coupled through the boundary conditions Equation (28) the tagged particle dynamics is not of renewal type.

3.1. Diagonalization of the Generator With the Coordinate Bethe Ansatz

Specifically, the backward generator $\hat{\mathcal{L}}^\dagger$ can be diagonalized exactly using the coordinate Bethe ansatz (see e.g., [67]). To that end we first require the solution of the separated (i.e., single particle) eigenvalue problem $\mathcal{L}_i^\dagger|\psi_{k_i}^L\rangle = -\lambda_{k_i}|\psi_{k_i}^L\rangle$ under the imposed external boundary conditions. Since $\varphi(x_{0,i}) = Fx_{0,i} + const$ we find that $p_{ss}(x_{0,i}) = \beta Fe^{-\beta Fx_{0,i}}(1-e^{-\beta F})^{-1}$ and because of the confinement we also have $\lambda_{0,i} = 0$ as well as $\psi_{0_i}^L(x_{0,i}) \equiv \langle x_{0,i}|\psi_{0_i}^L\rangle = 1$ and $\psi_{0_i}^R(x_{0,i}) \equiv \langle\psi_{0_i}^R|x_{0,i}\rangle = p_{ss}(x_{0,i})$. We are here interested in the role of particle number N and not of the magnitude of the force F, therefore we will henceforth set, for the sake of simplicity, $\beta F = D = 1$. The excited separated eigenvalues and eigenfunctions then read

$$\lambda_{k_i} = \pi^2 k_i^2 + \frac{1}{4},$$

$$\psi_{k_i}^L(x_{0,i}) = \frac{e^{x_{0,i}/2}}{(2\pi^2k_i^2+1/2)^{1/2}}\left(\sin(k_i\pi x_{0,i}) - 2k_i\pi\cos(k_i\pi x_{0,i})\right),$$

$$\forall k_i \in \mathbb{Z}^+, \tag{29}$$

with $\psi_{k_i}^R(x_{0,i}) = e^{-x_{0,i}}\psi_{k_i}^L(x_{0,i})$. It is straightforward to check that $\langle\psi_{k_i}^R|\psi_{l_i}^L\rangle = \delta_{k_i,l_i}$. Denoting by $\mathbf{k} = (k_i, k_2,\ldots,k_N)$ the N-tuple of all single-state indices k_i one can show by direct substitution that the many-body eigenvalues are given by $\lambda_\mathbf{k} = \sum_{i=1}^N \lambda_{k_i}$ and the corresponding orthonormal many-body eigenfunctions that obey the non-crossing internal boundary conditions Equation (28) have the form

$$\boldsymbol{\psi}_0^L(\mathbf{x}_0) = 1, \quad \boldsymbol{\psi}_0^R(\mathbf{x}_0) = N!\prod_{i=1}^N \frac{e^{-x_{0,i}}}{1-e^{-1}}$$

$$\boldsymbol{\psi}_\mathbf{k}^L(\mathbf{x}_0) = \sum_{\{k_i\}}\prod_{i=1}^N \psi_{k_i}^L(x_{0,i}), \boldsymbol{\psi}_\mathbf{k}^R(\mathbf{x}_0) = \mathbf{m_k}!\sum_{\{k_i\}}\prod_{i=1}^N \psi_{k_i}^R(x_{0,i}),$$

$$\tag{30}$$

where $\sum_{\{k_i\}}$ denotes the sum over all permutations of the elements of the N-tuple $\mathbf{k}$ and $\mathbf{m_k}! = \prod_i m_{k_i}!$ is the respective multiplicity of the eigenstate with m_{k_i} corresponding to the number of times a particular value of k_i appears in the tuple. It can be checked by explicit computation that the eigenfunctions defined in Equation (30) form a complete bi-orthonormal set, that is $\langle\psi_\mathbf{k}^R|\psi_\mathbf{l}^L\rangle = \delta_{\mathbf{k},\mathbf{l}}$ and $\sum_\mathbf{k}\boldsymbol{\psi}_\mathbf{k}^L(\mathbf{x}_0)\boldsymbol{\psi}_\mathbf{k}^R(\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x}_0)$.

3.2. Projection-Induced Non-Markovian Tagged Particle Dynamics

In the case of single file dynamics the physically motivated projection corresponds to the dynamics of a tagged particle upon integrating out the dynamics of the remaining particles. As

before, we assume that the full system is prepared in a steady state. The projection operator for the dynamics of the j-th particle is therefore defined as

$$\hat{\mathcal{P}}_{\mathbf{x}}(\delta; q_j) = \int_{\Xi} d\mathbf{x}\delta(x_j - q_j) = \left[\hat{O}\prod_{i=1}^{N}\int_0^1 dx_i\right]\delta(x_j - q_j), \quad (31)$$

where the operator $\hat{O}$ orders the integration limits $\int_0^1 dx_N \int_0^{x_N} dx_{N-1}\cdots \int_0^{x_2} dx_1$ since the domain Ξ is a hypercone. Here, the projection is from $\mathbb{R}^N$ to $\mathbb{R}$. Integrals of this kind are easily solvable with the so-called 'extended phase-space integration' [62, 87]. The non-Markovian Green's function is defined as

$$Q(q_j, t|q_{0,j}) = \frac{\hat{\mathcal{P}}_{\mathbf{x}}(\delta; q_j)\hat{\mathcal{P}}_{\mathbf{x}_0}(\delta; q_{0,j})G(\mathbf{x}, t|\mathbf{x}_0)p_{\mathrm{ss}}(\mathbf{x}_0)}{\hat{\mathcal{P}}_{\mathbf{x}_0}(\delta; q_{0,j})p_{\mathrm{ss}}(\mathbf{x}_0)} \quad (32)$$

and can be computed exactly according to Equation (10) to give

$$Q(q_j, t|q_{0,j}) = \Psi_{\mathbf{00}}(q_{0,j})^{-1}\sum_{\mathbf{k}}\Psi_{\mathbf{0k}}(q_j)\Psi_{\mathbf{k0}}(q_{0,j})e^{-\lambda_{\mathbf{k}}t}, \quad (33)$$

where the sum is over all Bethe eigenstates. If we denote the number of left and right neighbors by $N_L = (N - j + 1)$ and $N_R = j - 1$, respectively, all terms in Equation (33) read explicitly

$$\Psi_{\mathbf{00}}(q_j) = \frac{N!}{N_L!N_R!(1 - \mathrm{e}^{-1})^N}\mathrm{e}^{-q_j}(1 - \mathrm{e}^{-q_j})^{N_L}(\mathrm{e}^{-q_j} - \mathrm{e}^{-1})^{N_R}$$

$$\Psi_{\mathbf{k0}}(q_j) = \frac{N!}{N_L!N_R!(1 - \mathrm{e}^{-1})^N}\sum_{\{k_i\}}T(q_j)\prod_{i=1}^{j-1}L(q_j)\prod_{i=j+1}^{N}R(q_j) \quad (34)$$

and $\Psi_{\mathbf{0k}}(q_j) \equiv \Psi_{\mathbf{k0}}^{\dagger}(q_j) = \frac{\mathbf{m_k}!(1-\mathrm{e}^{-1})^N}{N!}\Psi_{\mathbf{k0}}(q_j)$. In Equation (34) we have introduced the auxiliary functions

$$T(q_j) = \delta_{\lambda_j, 0}\mathrm{e}^{-q_j} + (1 - \delta_{\lambda_j, 0})\frac{\mathrm{e}^{-q_j/2}}{\sqrt{1/2 + 2\pi^2\lambda_j^2}}$$
$$\left(\sin(\lambda_j\pi q_j) - 2\lambda_j\pi\cos(\lambda_j\pi q_j)\right)$$

$$L(q_j) = \delta_{\lambda_j, 0}(1 - \mathrm{e}^{-q_j}) - 2(1 - \delta_{\lambda_j, 0})\frac{\mathrm{e}^{-q_j/2}\sin(\lambda_j\pi q_j)}{\sqrt{1/2 + 2\pi^2\lambda_j^2}}$$

$$R(q_j) = \delta_{\lambda_j, 0}(\mathrm{e}^{-q_j} - \mathrm{e}^{-1}) + 2(1 - \delta_{\lambda_j, 0})\frac{\mathrm{e}^{-q_j/2}\sin(\lambda_j\pi q_j)}{\sqrt{1/2 + 2\pi^2\lambda_j^2}}$$
$$(35)$$

To the best of our knowledge, Equations (33) to (35) delivering the exact non-Markovian Green's function for the dynamics of the j-th particle in a tilted single file of N particles, have not yet been derived before. Note that one can also show that $\int_0^1 dq_j\Psi_{\mathbf{0k}}(q_j)\Psi_{\mathbf{l0}}(q_j) \neq 0$ and hence the Chapman–Kolmogorov equation is violated in agreement with Equation (13) confirming that the tagged particle diffusion is indeed non-Markovian on time-scales $t \lesssim \lambda_{\mathbf{1}}^{-1}$.

3.3. Markovian Approximation and Degree of Broken Markovianity

Since the projection leaves the coordinates untransformed the effective Markovian approximation in Equation (23) is particularly simple and corresponds to diffusion in the presence of an effective force deriving from the free energy of the tagged particle upon integrating out all the remaining particles assumed to be in equilibrium $\langle F(q_j)\rangle_{\mathbf{x}''} = -\langle \beta DF\delta(x_j - q_j)\rangle_{\mathbf{x}''}$ or, since $-\beta DFp_{\mathrm{ss}}(\mathbf{x}) = \partial_{x_j}p_{\mathrm{ss}}(\mathbf{x})$, explicitly defined as

$$\langle F(q_j)\rangle_{\mathbf{x}''} = \frac{\int_{\Xi} d\mathbf{x}\delta(x_j - q_j)\partial_{x_j}p_{\mathrm{ss}}(\mathbf{x})}{\int_{\Xi} d\mathbf{x}\delta(x_j - q_j)p_{\mathrm{ss}}(\mathbf{x})} \equiv \frac{\partial_{q_j}\int_{\Xi} d\mathbf{x}\delta(x_j - q_j)p_{\mathrm{ss}}(\mathbf{x})}{\int_{\Xi} d\mathbf{x}\delta(x_j - q_j)p_{\mathrm{ss}}(\mathbf{x})}.$$
$$(36)$$

Upon taking as before $D = \beta F = 1$, and noticing that $\Psi_{\mathbf{00}}(q_j) = \int_{\Xi} d\mathbf{x}\delta(x_j - q_j)p_{\mathrm{ss}}(\mathbf{x})$ we find

$$\langle\hat{\mathcal{L}}\rangle_{\mathbf{q}''} = \partial_{q_j}^2 + \partial_{q_j}\left\{\partial_{q_j}\ln\Psi_{\mathbf{00}}(q_j)\right\},$$
$$\langle\hat{\mathcal{L}}^{\dagger}\rangle_{\mathbf{q}''} = \partial_{q_j}^2 - \left\{\partial_{q_j}\ln\Psi_{\mathbf{00}}(q_j)\right\}\partial_{q_j} \quad (37)$$

where the curly bracket $\{\cdot\}$ denotes that the operator inside the bracket only acts within the bracket. The Markovian approximation of the Green's function thus becomes $Q_M(q_j, t|q_{0,j}) = \langle q_{0,j}|\mathrm{e}^{\langle\hat{\mathcal{L}}^{\dagger}\rangle_{\mathbf{x}''}t}|q_j\rangle$ and is to be compared to the exact non-Markovian Green's function (33) via the Kullback–Leibler divergence in Equation (24).

Our focus here is to asses how the "degree" of the projection, i.e., $d = N$, $a = 1$ and thus $d - a = N - 1$ – the number of latent degrees of freedom (here positions of non-tagged particles) being integrated out affects the time-dependence of the Kullback–Leibler divergence. Since the Markovian generator cannot be diagonalized analytically we used a finite element numerical method cross-checked with Brownian dynamics simulations to calculate $Q_M(q_j, t|q_{0,j})$. The corresponding Kullback–Leibler divergence (24) was in turn calculated by means of a numerical integration. We present results for the time dependence $\mathcal{D}_t(Q||Q_M)$ in two different representations, the absolute (dimensionless) time t and in units of the average number of collisions $\tilde{t} = t/N^2$, tagging the third particle ($j = 3$). The reason to adopt this second choice as the natural physical time-scale is that collisions in fact establish the effective dynamics and hence a typical collision time sets the natural time-scale.

Before going into details we comment on the following. Because we start from the same initial condition for projected coordinate (i.e., tagged particle) in both, the non-Markovian and Markovian setting, it follows trivially that $\lim_{t\to 0}\mathcal{D}_t(Q||Q_M) = 0$. A zero $\mathcal{D}_t(Q||Q_M)$ would persist until the typical time of occurrence of the first collision event. This collision time is, however, much shorter than t/N^2 because we start from equilibrium initial conditions on the full, many-body level implying a continuous (Boltzmann-weighted) distribution of initial distances of the tagged particle to its nearest neighbors. Using a spectral expansion, however, such vanishingly short time-scales are very difficult to capture, i.e., it would require an astronomically large number of eigenstates, which is

computationally not feasible. Conversely, because the tagged-particle invariant measures are by definition the same for the single file and its Markovian approximation [i.e., $\Psi_{00}(q_j)$ is equal for both; the first of Equation (34) enters Equation (37)], it also follows that $\lim_{t\to\infty} \mathcal{D}_t(Q||Q_M) = 0$. The relaxation time λ_1^{-1} in the many-body problem corresponds to the exploration of the entire system of length L (here set to unity); for further details see [67]. For a finite single file deviations from Markovianity are therefore transient, starting at zero, passing through a maximum, and decaying back to zero at times longer than the relaxation time λ_1^{-1} of the full, many-body model.

The results for $\mathcal{D}_t(Q||Q_M)$ for intermediate and long times are shown in **Figure 2**. From **Figure 2**, we confirm that the Markovianity is broken transiently (on time-scales $t \lesssim \lambda_1^{-1}$, which holds for any ergodic dynamics in the sense of generating an invariant measure. Notably, the relaxation time λ_1 does *not* depend on N and is hence equal for all cases considered here. Moreover, as expected, the magnitude of broken Markovianity increases with the "degree" of the projection (here with the particle number N), as is best seen on a natural time-scale (see **Figure 2B**). Conversely, on the absolute time-scale the relaxation rate of the Markovian approximation, describing diffusion on a free energy landscape $f(q_3) = -\beta \ln \Psi_{00}(q_3)$, which can be defined as

$$\lambda_1^M = -\lim_{t\to\infty} t^{-1} \ln(Q_M(q_j,t|q_{0,j}) - \Psi_{00}(q_j)) \qquad (38)$$

increases with increasing N (see inset in **Figure 2B**). Therefore, while both have by construction the same invariant measure, the Markovian approximation overestimates the rate of relaxation. This highlights the pitfall in using free energy landscape ideas in absence of a time-scale separation.

3.4. Tagged Particle Local Times Probing the Origin of Broken Markovianity

In order to gain deeper insight into the origin and physical meaning of memory emerging from integrating out latent degrees of freedom we inspect how a given tagged particle explores the configuration space starting from a stationary (equilibrium) initial condition. To that end we first compute the variance of local time of a tagged particle, $\theta_t(q_j)$ in Equation (25), given in the general form in Equation (26), which applied to tagged particle diffusion in a tilted single file reads:
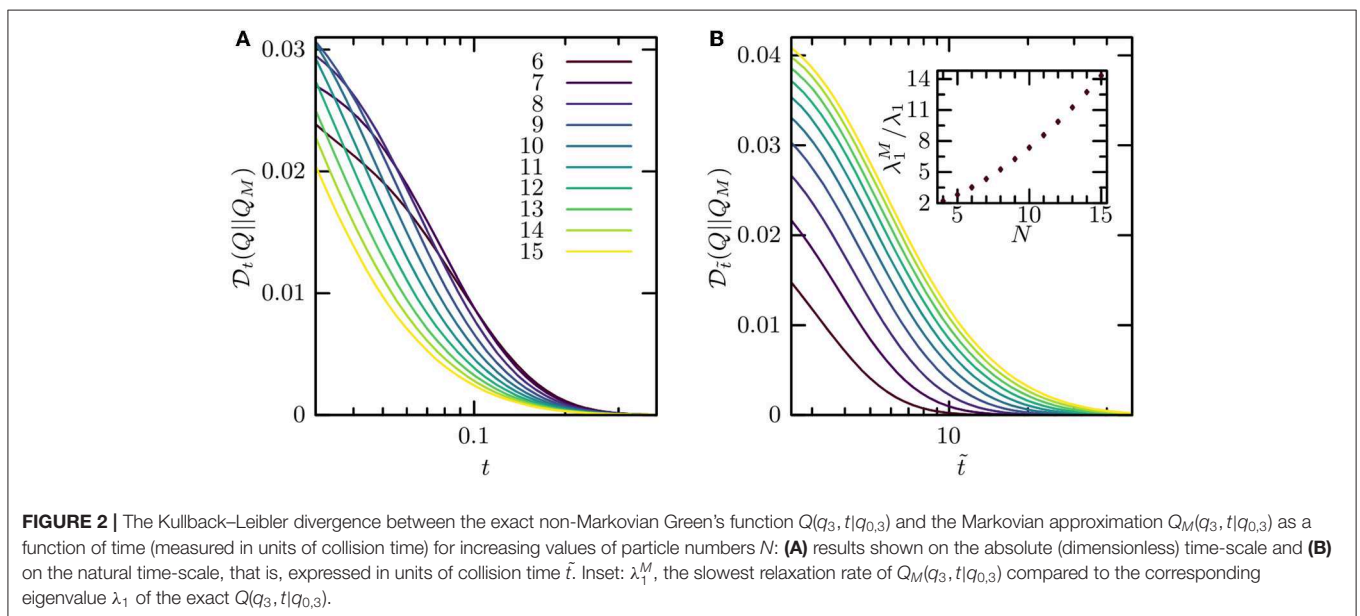
$$\sigma_t^2(q_j) = 2 \sum_k \frac{\Psi_{0k}(q_j)\Psi_{k0}(q_j)}{\lambda_k t} \left(1 - \frac{1 - e^{-\lambda_k t}}{\lambda_k t} \right) \qquad (39)$$

where $\Psi_{k0}(q_j)$ is given by Equation (34) and $\Psi_{0k}(q_j) = \frac{m_k!}{N!}\Psi_{k0}(q_j)$. Note that since the process in ergodic we have $\langle \theta_t(q_j) \rangle = \Psi_{00}(q_j)$, and because the projected dynamics becomes asymptotically Gaussian (i.e., the correlations between $\theta_t(q_j)$ at different t gradually decorrelate) we also have the large deviation $\lim_{t\to\infty} t\sigma_t^2(q_j) = 2\sum_k \lambda_k^{-1} \Psi_{0k}(q_j)\Psi_{k0}(q_j) \neq f(t)$. Moreover, because of detailed balance the large deviation principle represents an upper bound to fluctuations of time-average observables $\sigma_t^2(q_j) \leq 2\sum_k \frac{\Psi_{0k}(q_j)\Psi_{k0}(q_j)}{\lambda_k t}, \forall\, t$.

In order to gain more intuition we inspect the statistics of $\theta_t(q_j)$ for a single file of four particles (see **Figure 3**) at different lengths of trajectory t (plotted here on the absolute time-scale). In **Figure 3**, we show $\langle \theta_t(q_j) \rangle$ with full lines, and the region bounded by the standard deviation $\pm\sigma_t(q_j)$ with the shaded area.

The scatter of $\theta_t(q_j)$ is largest near the respective free energy minima.

To understand further how this coupling to non-relaxed latent degrees of freedom arises we inspect the correlations between
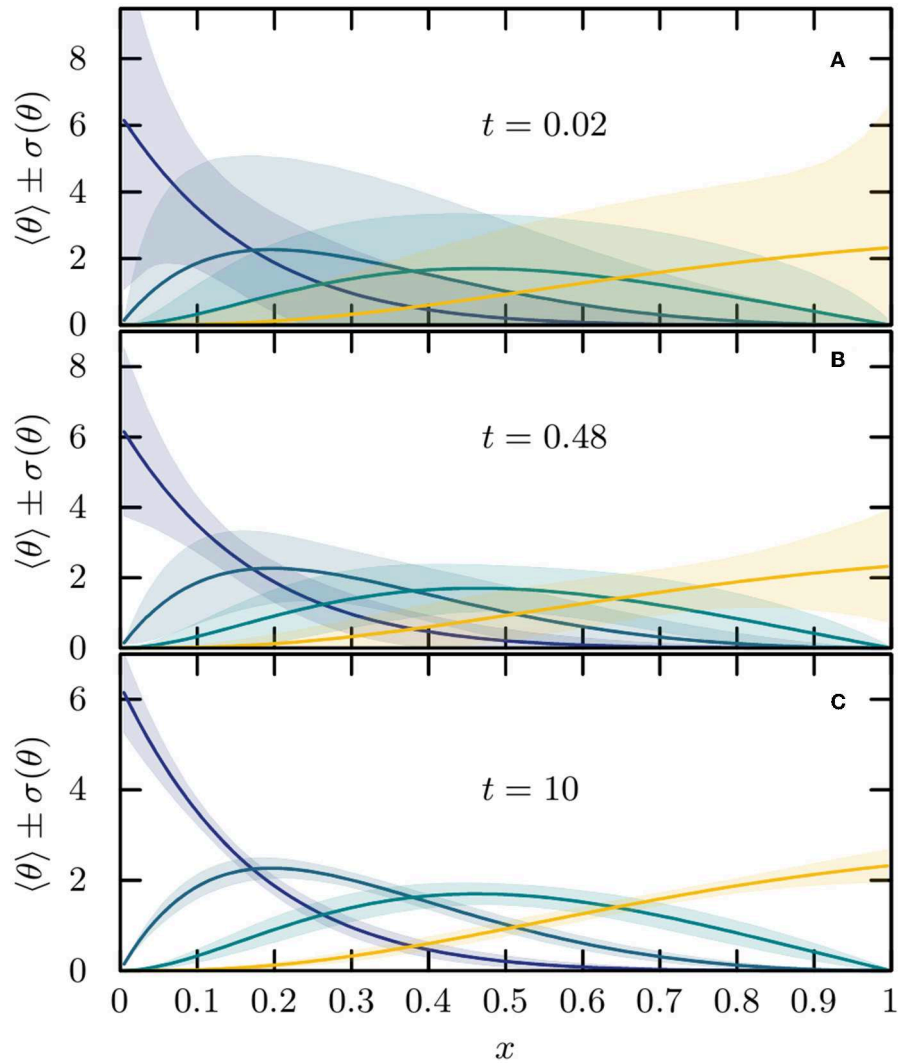

FIGURE 2 | The Kullback–Leibler divergence between the exact non-Markovian Green's function $Q(q_3,t|q_{0,3})$ and the Markovian approximation $Q_M(q_3,t|q_{0,3})$ as a function of time (measured in units of collision time) for increasing values of particle numbers N: **(A)** results shown on the absolute (dimensionless) time-scale and **(B)** on the natural time-scale, that is, expressed in units of collision time $\tilde{t}$. Inset: λ_1^M, the slowest relaxation rate of $Q_M(q_3,t|q_{0,3})$ compared to the corresponding eigenvalue λ_1 of the exact $Q(q_3,t|q_{0,3})$.

FIGURE 3 | Statistics of tagged particle local time for all members of a single file of four particles starting from stationary initial conditions; $\langle \theta_t(q_j) \rangle$ is represented by full lines and the region bounded by the standard deviation $\pm \sigma_t(q_j)$ with the corresponding shaded area. The color code is: $j = 1$ violet, $j = 2$ blue, $j = 3$, green and $j = 4$ yellow. The relaxation time corresponds to $\lambda_1^{-1} \simeq 0.1$. Therefore, panel **(A)** depicts fluctuations on a time scale much shorter that λ_1^{-1}, whereas **(B,C)** already belong deeply into the ergodic large deviation regime.

tagged particle histories

$$\mathcal{C}_t(q_i; q_j) = \sum_{\mathbf{k}} \frac{\Psi_{\mathbf{0k}}(q_i)\Psi_{\mathbf{k0}}(q_j) + \Psi_{\mathbf{0k}}(q_j)\Psi_{\mathbf{k0}}(q_i)}{\lambda_k t} \left(1 - \frac{1 - e^{-\lambda_k t}}{\lambda_k t} \right),$$

(40)

where as before $\lim_{t \to \infty} t\mathcal{C}_t(q_i; q_j) \equiv \overline{\mathcal{C}}_t(q_i; q_j) = \sum_{\mathbf{k}} \lambda_{\mathbf{k}}^{-1}(\Psi_{\mathbf{0k}}(q_i)\Psi_{\mathbf{k0}}(q_j) + \Psi_{\mathbf{0k}}(q_j)\Psi_{\mathbf{k0}}(q_i)) \neq f(t)$ as a manifestation of the central limit theorem, since $\theta_t(q_i)$ and $\theta_t(q_j)$ asymptotically decorrelate. In other words, taking $\mathcal{C}_t(q_i; q_i) \equiv \sigma_t^2(q_i)$, the complete large deviation statistics of $\theta_t(q_i)$ (i.e., on ergodically long time-scales) is a N-dimensional Gaussian with covariance matrix $t^{-1}\overline{\mathcal{C}}_t(q_i; q_j)$.

To visualize these results we present in **Figures 4**, **5** two-tag nearest neighbor and next-nearest correlations, $\mathcal{C}_t(q_1; q_3)$ and as $\mathcal{C}_t(q_2; q_3)$ respectively, for a single file of $N = 4$ and $N = 7$ particles at two different trajectory lengths. We find that, alongside the fact that correlations intuitively increase with the N, both the magnitude and the sign of $\mathcal{C}_t$ depend on which particles we tag and even more so, where we tag these particles. Along the (upward shifted) diagonal $\mathcal{C}_t$ is positive, implying the two tagged particles along a stochastic many-body trajectory effectively (in the sense of the local time) move together, such that if one particle spends more time in a given region, so will the other. At fixed F (here assumed to be equal to 1) the magnitude of the upward shift depends on which particles we tag as well as on N. This
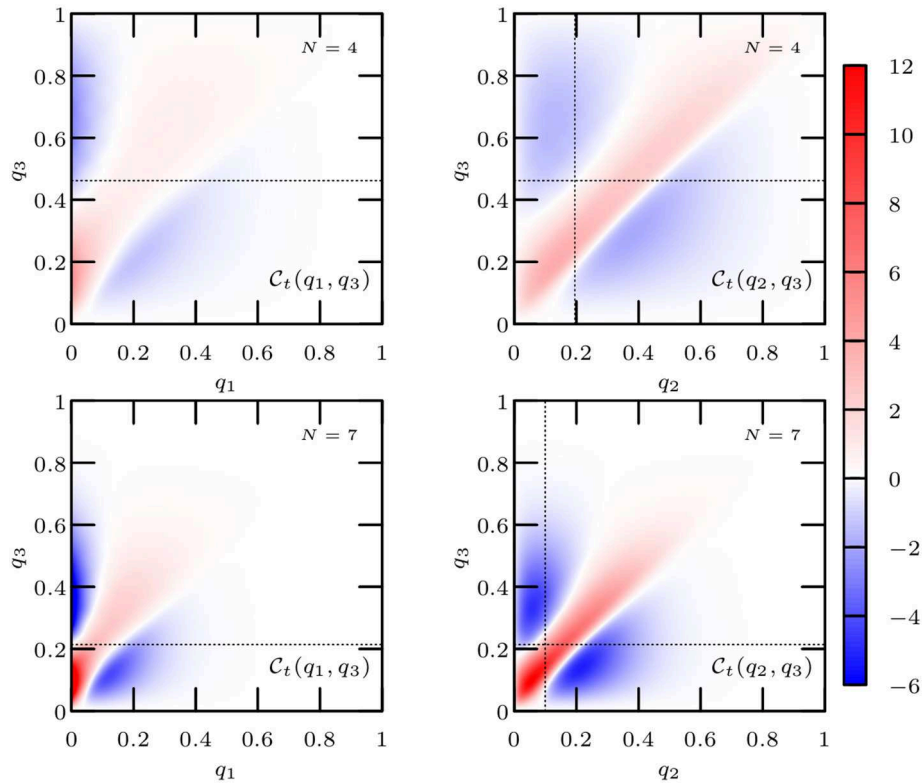
FIGURE 4 | Two-tag local time correlations $\mathcal{C}_t(q_1; q_3)$ **(left)** and $\mathcal{C}_t(q_2; q_3)$ **(right)** for a single file of $N = 4$ **(top)** and $N = 7$ **(bottom)** particles for a (very short) trajectory length $t = 0.01$. The relaxation time corresponds to $\lambda_1^{-1} \simeq 0.1$. The dashed lines denote the positions of the two free energy minima.

intuitive idea is backed up mathematically by realizing that the lowest excited Bethe-eigenfunctions correspond to collective ("in phase") motion (see Equations 29, 30). Furthermore, defining the free energy minima of the tagged particles with $q_i^{\min}$ and $q_i^{\min}$ (see dashed lines in **Figures 4**, **5**) we would expect, if the particles were to explore their respective free energy minima, a peak localized at $(q_i^{\min}, q_i^{\min})$ (i.e., at the crossing of dashed line in **Figures 4**, **5**). We find, however, that this is not the case, all together implying that the *tagged particles do not, along a many-body trajectory, explore their respective free energy minima*. Instead, as mentioned above, they move collectively close to each other. The collective dynamics is therefore non-trivial and the tagged particle dynamics cannot be, at least for $t \lesssim \lambda_1^{-1}$ coarse grained to a Markovian diffusion on $-\beta \ln \Psi_{00}(q_j)$, the free energy landscape of the tagged particle j. Conversely, the fact that all correlations (positive and negative) die our as $q_{i,j} \to 1$ is a straightforward consequence of the tilting of the confining box.

Focusing now on the dependence on the length of the trajectory we see at very short time (much shorter than the relaxation time) the correlations are stronger, and that positive correlations peak further away from the two respective tagged particle free energy minima (compare **Figure 4** and **Figure 5**). In addition, the maximum of $\mathcal{C}_t(q_i; q_j)$ appears to be somewhat more localized at longer (nearly ergodic) times (see **Figure 5**). In addition, the tagged particle dynamics seem to be localized more strongly near the free energy minimum if we tag the first particle

and if N is larger, presumably because of a faster relaxation due to the presence of the wall effecting more frequent collisions with the wall, during which the particle eventually loses memory.

4. SUMMARY AND OUTLOOK

Non-Markovian dynamics and anomalous diffusion are particularly ubiquitous and important in biophysical systems [1–16]. There, however, it appears that the quite many non-Markovian observations are described theoretically by phenomenological approaches with *ad-hoc* memory kernels, which in specific cases can lead to mathematically unsound or even unphysical behavior [82]. It therefore seems timely and useful to provide a theoretical perspective of non-Markovian dynamics starting from more fine-grained principles and considering a projection to some effective lower-dimensional configuration space.

The ideas presented here are neither new nor completely general. Projection-operator concepts date back to the original works by Zwanzig, Mori, Nakajima, van Kampen, Hänggi and other pioneers. However, these seminal contributions focused mostly on the derivation and analysis of effective non-Markovian evolution operators, whereas here we provide a thorough analysis of the manifestations of the projection on the level of Green's functions with the aim to somewhat relieve the need for choosing a particular model based solely on physical intuition.
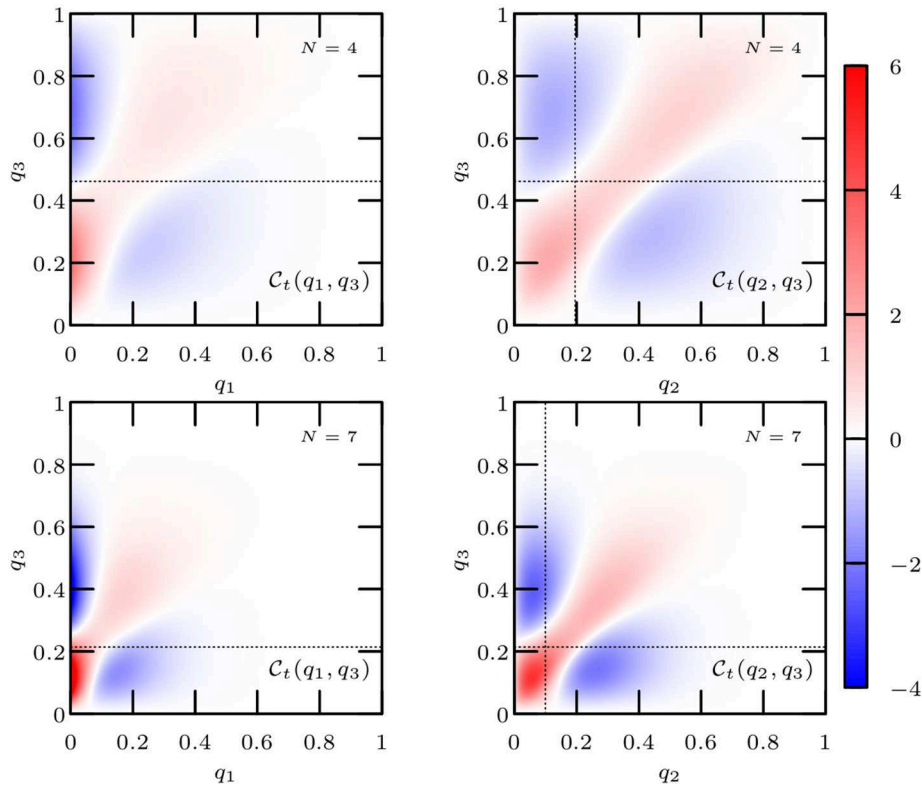
FIGURE 5 | Two-tag local time correlations $\mathcal{C}_t(q_1; q_3)$ **(left)** and $\mathcal{C}_t(q_2; q_3)$ **(right)** for a single file of $N = 4$ **(top)** and $N = 7$ **(bottom)** particles for a trajectory length comparable to the relaxation time $t = 0.12 \simeq \lambda_1^{-1}$. The relaxation time corresponds to $\lambda_1^{-1} \simeq 0.1$. The dashed lines denote the positions of the two free energy minima.

Furthermore, we rigorously establish conditions under which the projected dynamics become Markovian and renewal-type, and derive Markovian approximations to projected generators. As a diagnostic tool we propose a novel framework for the assessment of the degree of broken Markovianity as well as for the elucidation of the origins of non-Markovian behavior.

An important remark concerns the transience of broken Markovianity, which is a consequence of the fact that we assumed that the complete dynamics is ergodic. First we note that (i) for any finite observation of length t it is *de facto* not possible to discern whether the observation (and the dynamics in general) will be ergodic or not on a time scale $\tau > t$. (ii) All physical observations are (trivially) finite. (iii) In a nominally ergodic dynamics on any finite time scale t, where the dynamics starting from some non-stationary initial condition $\mathbf{x}_0$ has not yet reached the steady state (in the language of this work $t < \lambda_1^{-1}$), it is not possible to observe the effect of a sufficiently distant confining boundary $\partial\Omega(\mathbf{x})$ (potentially located at infinity if the drift field $\mathbf{F}(\mathbf{x})$ is sufficiently confining) that would assure ergodicity (in the language of this work $\forall t \ll \lambda_1^{-1}$ such that $G(l_{\min}, t | \mathbf{x}_0, 0) \simeq 0$ where $|l_{\min}| \equiv \min_{\mathbf{x}} |\mathbf{x}_0 - \partial\Omega(\mathbf{x})|$). Therefore *no generality is lost in our work by assuming that the complete dynamics is nominally ergodic*, even in a rigorous treatment of so-called weakly non-ergodic dynamics with diverging mean waiting times (see e.g., [1, 6]) or generalized Langevin dynamics with diverging

correlation times (see e.g., [29–34]) on finite time-scales. As a corollary, in the description of such dynamics on any finite time-scale it is *a priori* by no means necessary to assume that the dynamics is non-ergodic or has a diverging correlation time. This does not imply, however, that the assumption of diverging mean waiting times or diverging correlation times cannot render the analysis of specific models simpler.

Notably, our work considers parent dynamics with a potentially broken time-reversal symmetry and hence includes the description of projection-induced non-Markovian dynamics in non-equilibrium (i.e., irreversible) systems. In the latter case the relaxation process of the parent microscopic process might not be monotonic (i.e., may oscillate), and it will be very interesting to explore the manifestations and importance of these oscillations in projected non-Markovian dynamics.

In the context of renewal dynamics our work builds on firm mathematical foundations of Markov processes and therefore provides mathematically and physically consistent explicit (but notably not necessarily the most general) memory kernels derived from microscopic (or fine-grained) principles, which can serve for the development, assessment and fine-tuning of empirical memory kernels that are used frequently in the theoretical modeling of non-Markovian phenomena (e.g., power-law, exponential, stretched exponential etc; [2, 82]). In particular, power-law kernels are expected to emerge as transients

in cases, where the latent degrees of freedom relax over multiple time-scales with a nearly continuous and self-similar spectrum. Conversely, the quite strongly restrictive conditions imposed on the microscopic (parent) dynamics that lead to renewal dynamics, which we reveal here, suggest that renewal type transport in continuous space (e.g., continuous-time random walks [1, 2]) might not be the most abundant processes underlying projection-induced non-Markovian dynamics in physical systems, but are more likely to arise due to some disorder averaging. In general, it seems natural that coarse graining involving some degree of spatial discretization should underly renewal type ideas.

From a more general perspective beyond the theory of anomalous diffusion our results are relevant for the description and understanding of experimental observables $a(\mathbf{q})$ coupled to projected dynamics $\mathbf{q}(t)$ in presence of slow latent degrees of freedom (e.g., a FRET experiment measuring the distance within a protein or a DNA molecule [88]), as well as for exploring stochastic thermodynamic properties of projected dynamics with slow hidden degrees of freedom [89–91]. An important field of applications of the spectral-theoretic ideas developed here is the field of statistical kinetics in the context of first passage concepts (e.g., [92–94]), where general results for non-Markovian dynamics are quite sparse [46, 49, 95–100] and will be the subject of our future studies.

DATA AVAILABILITY STATEMENT

All datasets generated for this study are included in the article/supplementary material.

AUTHOR CONTRIBUTIONS

AL and AG conceived the research, performed the research, and wrote and reviewed the paper.

REFERENCES

1. Metzler R, Klafter J. The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Phys Rep.* (2000) **339**:1–77. doi: 10.1016/S0370-1573(00)00070-3
2. Metzler R, Klafter J. The restaurant at the end of the random walk: recent developments in the description of anomalous transport by fractional dynamics. *J Phys A Math Gen.* (2004) **37**:R161–208. doi: 10.1088/0305-4470/37/31/R01
3. Sokolov IM, Klafter J. From diffusion to anomalous diffusion: a century after Einstein's Brownian motion. *Chaos.* (2005) **15**:026103. doi: 10.1063/1.1860472
4. Klages R, Radons G, Sokolov IM. *Anomalous Transport: Foundations and Applications.* Weinheim: Wiley-VCH Verlag GmbH and Co. (2008).
5. Godec A, Bauer M, Metzler R. Collective dynamics effect transient subdiffusion of inert tracers in flexible gel networks. *N J Phys.* (2014) **16**:092002. doi: 10.1088/1367-2630/16/9/092002
6. Metzler R, Jepn JH, Cherstvy AG, Barkai E. Anomalous diffusion models and their properties: non-stationarity, non-ergodicity, and ageing at the centenary of single particle tracking. *Phys Chem Chem Phys.* (2014) **16**:24128–64. doi: 10.1039/C4CP03465A
7. Höfling F, Franosch T. Anomalous transport in the crowded world of biological cells. *Rep Prog Phys.* (2013) **76**:046602. doi: 10.1088/0034-4885/76/4/046602
8. Sokolov IM. Models of anomalous diffusion in crowded environments. *Soft Matter.* (2012) **8**:9043–52. doi: 10.1039/c2sm25701g
9. Metzler R, Jeon JH, Cherstvy AG. Non-Brownian diffusion in lipid membranes: experiments and simulations. *Biochim Biophys Acta Biomemb.* (2016) **1858**:2451–67. doi: 10.1016/j.bbamem.2016.01.022
10. Oliveira FA, Ferreira RMS, Lapas LC, Vainstein MH. Anomalous diffusion: a basic mechanism for the evolution of inhomogeneous systems. *Front Phys.* (2019) 7:18. doi: 10.3389/fphy.2019.00018
11. Woringer M, Darzacq X. *Protein Motion in the Nucleus: From Anomalous Diffusion to Weak Interactions.* Biochemical Society Transactions (2018). Available online at: http://www.biochemsoctrans.org/content/early/2018/07/29/BST20170310
12. Dix JA, Verkman AS. Crowding effects on diffusion in solutions and cells. *Annu Rev Biophys.* (2008) **37**:247–63. doi: 10.1146/annurev.biophys.37.032807.125824
13. Krapf D. Chapter 5: Mechanisms underlying anomalous diffusion in the plasma membrane. In: Kenworthy AK, editor. *Lipid Domains. Vol. 75 of Current Topics in Membranes.* Academic Press (2015). p. 167–207.
14. Golding I, Cox EC. Physical nature of bacterial cytoplasm. *Phys Rev Lett.* (2006) **96**:098102. doi: 10.1103/PhysRevLett.96.098102
15. Jeon JH, Javanainen M, Martinez-Seara H, Metzler R, Vattulainen I. Protein crowding in lipid bilayers gives rise to non-Gaussian anomalous lateral diffusion of phospholipids and proteins. *Phys Rev X.* (2016) **6**:021006. doi: 10.1103/PhysRevX.6.021006
16. Rienzo CD, Piazza V, Gratton E, Beltram F, Cardarelli F. Probing short-range protein Brownian motion in the cytoplasm of living cells. *Nat Commun.* (2014) 5:5891. doi: 10.1038/ncomms6891
17. Metzler R, Klafter J. Anomalous stochastic processes in the fractional dynamics framework: fokker:planck equation, dispersive transport, and non?exponential relaxation. In: Prigogine I and Rice SA editors. *Advances in Chemical Physics*, Vol 116. JohnWiley and Sons, Ltd (2007). doi: 10.1002/9780470141762.ch3
18. Lomholt MA, Lizana L, Metzler R, Ambjörnsson T. Microscopic origin of the logarithmic time evolution of aging processes in complex systems. *Phys Rev Lett.* (2013) **110**:208301. doi: 10.1103/PhysRevLett.110.208301
19. Bouchaud JP, Georges A. Anomalous diffusion in disordered media: statistical mechanisms, models and physical applications. *Phys Rep.* (1990) **195**:127–93.
20. Bouchaud JP, Comtet A, Georges A, Doussal PL. Classical diffusion of a particle in a one-dimensional random force field. *Ann Phys.* (1990) **201**:285–341.
21. Sinai YG. The limiting behavior of a one-dimensional random walk in a random medium. *Theory Prob Appl.* (1982) **27**:285–341.

22. Oshanin G, Rosso A, Schehr G. Anomalous fluctuations of currents in sinai-type random chains with strongly correlated disorder. *Phys Rev Lett.* (2013) **110**:100602. doi: 10.1103/PhysRevLett.110.100602

23. Dean DS, Gupta S, Oshanin G, Rosso A, Schehr G. Diffusion in periodic, correlated random forcing landscapes. *J Phys A Math Theor.* (2014) **47**:372001. doi: 10.1088/1751-8113/47/37/372001

24. Radons G. Anomalous transport in disordered dynamical systems. *Phys D Nonlinear Phenomena.* (2004) **187**:3–19. doi: 10.1016/j.physd.2003.09.001

25. Godec A, Chechkin AV, Barkai E, Kantz H, Metzler R. Localisation and universal fluctuations in ultraslow diffusion processes. *J Phys A Math Theor.* (2014) **47**:492002. doi: 10.1088/1751-8113/47/49/492002

26. Krüsemann H, Godec A, Metzler R. First-passage statistics for aging diffusion in systems with annealed and quenched disorder. *Phys Rev E.* (2014) **89**:040101. doi: 10.1103/PhysRevE.89.040101

27. Krsemann H, Godec A, Metzler R. Ageing first passage time density in continuous time random walks and quenched energy landscapes. *J Phys A Math Theor.* (2015) **48**:285001. doi: 10.1088/1751-8113/48/28/285001

28. Coffey WT, Kalmykov YP, Waldron JT. *The Langevin Equation.* World Scientific (1996). Available online at: https://www.worldscientific.com/doi/abs/10.1142/2256

29. Jeon JH, Metzler R. Fractional Brownian motion and motion governed by the fractional Langevin equation in confined geometries. *Phys Rev E.* (2010) **81**:021103. doi: 10.1103/PhysRevE.81.021103

30. Lutz E. Fractional Langevin equation. *Phys Rev E.* (2001) **64**:051106. doi: 10.1103/PhysRevE.64.051106

31. Deng W, Barkai E. Ergodic properties of fractional Brownian-Langevin motion. *Phys Rev E.* (2009) **79**:011112. doi: 10.1103/PhysRevE.79.011112

32. Metzler R, Klafter J. Subdiffusive transport close to thermal equilibrium: From the Langevin equation to fractional diffusion. *Phys Rev E.* (2000) **61**:6308–11. doi: 10.1103/PhysRevE.61.6308

33. Kou SC, Xie XS. Generalized Langevin equation with fractional Gaussian noise: subdiffusion within a single protein molecule. *Phys Rev Lett.* (2004) **93**:180603. doi: 10.1103/PhysRevLett.93.180603

34. Burov S, Barkai E. Critical exponent of the fractional Langevin equation. *Phys Rev Lett.* (2008) **100**:070601. doi: 10.1103/PhysRevLett.100.070601

35. Goychuk I. Viscoelastic subdiffusion: generalized langevin equation approach. In: Rice SA, Dinner AR editors. *Advances in Chemical Physics*, Vol 150. JohnWiley and Sons, Ltd (2012). doi: 10.1002/9781118197714.ch5

36. Dubkov AA, Hänggi P, Goychuk I. Non-linear Brownian motion: the problem of obtaining the thermal Langevin equation for a non-Gaussian bath. *J Stat Mech Theory Exp.* (2009) (2009) 2009:P01034. doi: 10.1088/1742-5468/2009/01/P01034

37. Cherstvy AG, Chechkin AV, Metzler R. Anomalous diffusion and ergodicity breaking in heterogeneous diffusion processes. *N J Phys.* (2013) **15**:083039. doi: 10.1088/1367-2630/15/8/083039

38. Cherstvy AG, Metzler R. Nonergodicity, fluctuations, and criticality in heterogeneous diffusion processes. *Phys Rev E.* (2014) **90**:012134. doi: 10.1103/PhysRevE.90.012134

39. Massignan P, Manzo C, Torreno-Pina JA, García-Parajo MF, Lewenstein M, Lapeyre GJ. Nonergodic subdiffusion from Brownian motion in an inhomogeneous medium. *Phys Rev Lett.* (2014) **112**:150603. doi: 10.1103/PhysRevLett.112.150603

40. Guérin T, Dean DS. Force-induced dispersion in heterogeneous media. *Phys Rev Lett.* (2015) **115**:020601. doi: 10.1103/PhysRevLett.115.020601

41. Godec A, Metzler R. Optimization and universality of Brownian search in a basic model of quenched heterogeneous media. *Phys Rev E.* (2015) **91**:052134. doi: 10.1103/PhysRevE.91.052134

42. Vaccario G, Antoine C, Talbot J. First-passage times in *d*-dimensional heterogeneous media. *Phys Rev Lett.* (2015) **115**:240601. doi: 10.1103/PhysRevLett.115.240601

43. Godec A, Metzler R. First passage time distribution in heterogeneity controlled kinetics: going beyond the mean first passage time. *Sci Rep.* (2016) **6**:20349. doi: 10.1038/srep20349

44. Chubynsky MV, Slater GW. Diffusing diffusivity: a model for anomalous, yet Brownian, diffusion. *Phys Rev Lett.* (2014) **113**:098302. doi: 10.1103/PhysRevLett.113.098302

45. Chechkin AV, Seno F, Metzler R, Sokolov IM. Brownian yet non-Gaussian diffusion: from superstatistics to subordination of diffusing diffusivities. *Phys Rev X.* (2017) **7**:021002. doi: 10.1103/PhysRevX.7.021002

46. Godec A, Metzler R. First passage time statistics for two-channel diffusion. *J Phys A Math Theor.* (2017) **50**:084001. doi: 10.1088/1751-8121/aa5204

47. Sposini V, Chechkin AV, Seno F, Pagnini G, Metzler R. Random diffusivity from stochastic equations: comparison of two models for Brownian yet non-Gaussian diffusion. *N J Physics.* (2018) **20**:043044. doi: 10.1088/1367-2630/aab696

48. Lanoiselée Y, Grebenkov DS. A model of non-Gaussian diffusion in heterogeneous media. *J Phys A Math Theor.* (2018) **51**:145602. doi: 10.1088/1751-8121/aab15f

49. Grebenkov DS. A unifying approach to first-passage time distributions in diffusing diffusivity and switching diffusion models. *J Phys A Math Theor.* (2019) **52**:174001. doi: 10.1088/1751-8121/ab0dae

50. Lanoiselee Y, Moutal N, Grebenkov DS. Diffusion-limited reactions in dynamic heterogeneous media. *Nat Commun.* (2018) **9**:4398. doi: 10.1038/s41467-018-06610-6

51. Zwanzig R. Ensemble method in the theory of irreversibility. *J Chem Phys.* (1960) **33**:1338–41. doi: 10.1063/1.1731409

52. Nordholm S, Zwanzig R. A systematic derivation of exact generalized Brownian motion theory. *J Stat Phys.* (1975) **13**:347–71. doi: 10.1007/BF01012013

53. Mori H. Transport, collective motion, and Brownian motion*). *Prog Theor Phys.* (1965) **33**:423–55. doi: 10.1143/PTP.33.423

54. Grabert H, Talkner P, Hänggi P. Microdynamics and time-evolution of macroscopic non-Markovian systems. *Z B Condensed Matter.* (1977) **26**:389–95. doi: 10.1007/BF01570749

55. Hänggi P, Thomas H. Time evolution, correlations, and linear response of non-Markov processes. *Z Condensed Matter.* (1977) **26**:85–92. doi: 10.1007/BF01313376

56. Grabert H, Talkner P, Hänggi P, Thomas H. Microdynamics and time-evolution of macroscopic non-Markovian systems. II. *Z B Condensed Matter.* (1978) **29**:273–80. doi: 10.1007/BF01321192

57. Hynes JT, Kapral R, Weinberg M. Microscopic theory of Brownian motion: mori friction kernel and Langevin-equation derivation. *Phys A Stat Mech Appl.* (1975) **80**:105–27.

58. Haken H. Cooperative phenomena in systems far from thermal equilibrium and in nonphysical systems. *Rev Mod Phys.* (1975) **47**:67–121. doi: 10.1103/RevModPhys.47.67

59. Ferrario M, Grigolini P. The non-Markovian relaxation process as a "contraction" of a multidimensional one of Markovian type. *J Math Phys.* (1979) **20**:2567–72. doi: 10.1063/1.524019

60. Grigolini P. A Fokker-Planck equation for canonical non-Markovian systems: a local linearization approach. *J Chem Phys.* (1988) **89**:4300–8. doi: 10.1063/1.454812

61. Harris TE. Diffusion with "collisions" between particles. *J Appl Probab.* (1965) **2**:323–38.

62. Lizana L, Ambjörnsson T. Single-file diffusion in a box. *Phys Rev Lett.* (2008) **100**:200601. doi: 10.1103/PhysRevLett.100.200601

63. Barkai E, Silbey R. Theory of single file diffusion in a force field. *Phys Rev Lett.* (2009) **102**:050602. doi: 10.1103/PhysRevLett.102.050602

64. Sanders LP, Lomholt MA, Lizana L, Fogelmark K, Metzler R, Ambjrnsson T. Severe slowing-down and universality of the dynamics in disordered interacting many-body systems: ageing and ultraslow diffusion. *N J Phys.* (2014) **16**:113050. doi: 10.1088/1367-2630/16/11/113050

65. Illien P, Bénichou O, Mejía-Monasterio C, Oshanin G, Voituriez R. Active transport in dense diffusive single-file systems. *Phys Rev Lett.* (2013) **111**:038102. doi: 10.1103/PhysRevLett.111.038102

66. Bertrand T, Illien P, Bénichou O, Voituriez R. Dynamics of run-and-tumble particles in dense single-file systems. *N J Phys.* (2018) **20**:113045. doi: 10.1088/1367-2630/aaef6f

67. Lapolla A, Godec A. Unfolding tagged particle histories in single-file diffusion: exact single- and two-tag local times beyond large deviation theory. *N J Phys.* (2018) **20**:113021. doi: 10.1088/1367-2630/aaea1b

68. Godec A, Metzler R. Signal focusing through active transport. *Phys Rev E.* (2015) **92**:010701. doi: 10.1103/PhysRevE.92.010701

69. Deutch JM, Silbey R. Exact generalized Langevin equation for a particle in a harmonic lattice. *Phys Rev A.* (1971) **3**:2049–52. doi: 10.1103/PhysRevA.3.2049

70. Havlin S, Kiefer JE, Weiss GH. Anomalous diffusion on a random comblike structure. *Phys Rev A.* (1987) **36**:1403–8. doi: 10.1103/PhysRevA.36.1403

71. Pottier N. Analytic study of a model of diffusion on random comb-like structures. *Il Nuovo Cimento D.* (1994) **16**:1223–30. doi: 10.1007/BF02458804

72. Berezhkovskii AM, Dagdug L, Bezrukov SM. From normal to anomalous diffusion in comb-like structures in three dimensions. *J Chem Phys.* (2014) **141**:054907. doi: 10.1063/1.4891566

73. Qian H. A decomposition of irreversible diffusion processes without detailed balance. *J Math Phys.* (2013) **54**:053302. doi: 10.1063/1.4803847

74. Gray AH. Uniqueness of steady-state solutions to the Fokker-Planck equation. *J Math Phys.* (1965) **6**:644–7. doi: 10.1063/1.1704316

75. Huang W, Ji M, Liu Z, Yi Y. Steady states of Fokker–Planck equations: I. existence. *J Dyn Diff Equ.* (2015) **27**:721–42. doi: 10.1007/s10884-015-9454-x

76. Helffer B, Nier F. *Hypoelliptic Estimates and Spectral Theory for Fokker-Planck Operators and Witten Laplacians.* Berlin; Heidelberg: Springer (2005).

77. Chupin L. Fokker-Planck equation in bounded domain. *Ann Inst Fourier.* (2010) **60**:217. doi: 10.5802/aif.2521

78. Reed M, Simon B. *Methods of Modern Mathematical Physics I: Functional Analysis.* New York, NY: Academic Press (1972).

79. Conway JB. *A Course in Functional Analysis.* New York, NY: Springer-Verlag (1985).

80. Feller W. Non-Markovian processes with the semigroup property. *Ann Math Statist.* (1959) **30**:1252–3. doi: 10.1214/aoms/1177706110

81. Hanggi P, Thomas H, Grabert H, Talkner P. Note on time evolution of non-Markov processes. *J Stat Phys.* (1978) **18**:155–9. doi: 10.1007/BF01014306

82. Sokolov IM. Solutions of a class of non-Markovian Fokker-Planck equations. *Phys Rev E.* (2002) **66**:041101. doi: 10.1103/PhysRevE.66.041101

83. Risken H, Haken H. *The Fokker-Planck Equation: Methods of Solution and Applications.* 2nd ed. Springer (1989).

84. Polettini M. Generally covariant state-dependent diffusion. *J Stat Mech Theory Exp.* (2013) **2013**:P07005. doi: 10.1088/1742-5468/2013/07/P07005

85. Polettini M, Esposito M. Nonconvexity of the relative entropy for Markov dynamics: a Fisher information approach. *Phys Rev E.* (2013) **88**:012112. doi: 10.1103/PhysRevE.88.012112

86. Korepin VE, Bogoliubov NM, Izergin AG. *Quantum Inverse Scattering Method and Correlation Functions.* Cambridge University Press (1993). doi: 10.1017/CBO9780511628832

87. Lizana L, Ambjörnsson T. Diffusion of finite-sized hard-core interacting particles in a one-dimensional box: tagged particle dynamics. *Phys Rev E.* (2009) **80**:051103. doi: 10.1103/PhysRevE.80.051103

88. Gopich IV, Szabo A. Theory of the energy transfer efficiency and fluorescence lifetime distribution in single-molecule FRET. *Proc Natl Acad Sci USA.* (2012) **109**:7747–52. doi: 10.1073/pnas.1205120109

89. Seifert U. Stochastic thermodynamics, fluctuation theorems and molecular machines. *Rep Prog Phys.* (2012) **75**:126001. doi: 10.1088/0034-4885/75/12/126001

90. Mehl J, Lander B, Bechinger C, Blickle V, Seifert U. Role of hidden slow degrees of freedom in the fluctuation theorem. *Phys Rev Lett.* (2012) **108**:220601. doi: 10.1103/PhysRevLett.108.220601

91. Uhl M, Pietzonka P, Seifert U. Fluctuations of apparent entropy production in networks with hidden slow degrees of freedom. *J Stat Mech Theory Exp.* (2018) **2018**:023203. doi: 10.1088/1742-5468/aaa78b

92. Hartich D, Godec A. Duality between relaxation and first passage in reversible Markov dynamics: rugged energy landscapes disentangled. *N J Phys.* (2018) **20**:112002. doi: 10.1088/1367-2630/aaf038

93. Hartich D, Godec A. Interlacing relaxation and first-passage phenomena in reversible discrete and continuous space Markovian dynamics. *J Stat Mech Theory Exp.* (2019) **2019**:024002. doi: 10.1088/1742-5468/ab00df

94. Hartich D, Godec A. Extreme value statistics of ergodic Markov processes from first passage times in the large deviation limit. *J Phys A Math Theor.* (2019) **52**:244001. doi: 10.1088/1751-8121/ab1eca

95. Hänggi P, Talkner P. Non-Markov processes: the problem of the mean first passage time. *Z B Condensed Matter.* (1981) **45**:79–83. doi: 10.1007/BF01294279

96. Balakrishnan V, Van den Broeck C, Hänggi P. First-passage times of non-Markovian processes: the case of a reflecting boundary. *Phys Rev A.* (1988) **38**:4213–22. doi: 10.1103/PhysRevA.38.4213

97. McKane AJ, Luckock HC, Bray AJ. Path integrals and non-Markov processes. I. General formalism. *Phys Rev A.* (1990) **41**:644–56. doi: 10.1103/PhysRevA.41.644

98. Reimann P, Schmid GJ, Hänggi P. Universal equivalence of mean first-passage time and Kramers rate. *Phys Rev E.* (1999) **60**:R1–4. doi: 10.1103/PhysRevE.60.R1

99. Bray AJ, Majumdar SN, Schehr G. Persistence and first-passage properties in nonequilibrium systems. *Adv Phys.* (2013) **62**:225–361. doi: 10.1080/00018732.2013.803819

100. Guerin T, Levernier N, Benichou O, Voituriez R. Mean first-passage times of non-Markovian random walkers in confinement. *Nature.* (2016) **534**:356–9. doi: 10.1038/nature18272

Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.