Single-file diffusion in a bi-stable potential: signatures of memory in the barrier-crossing of a tagged-particle

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We investigate memory effects in barrier-crossing in the overdamped setting. We focus on the scenario where the hidden degrees of freedom relax on exactly the same time scale as the observable. As a prototypical model we analyze tagged-particle diffusion in a single-file confined to a bi-stable potential. We identify the signatures of memory and explain their origin. The emerging memory is a result of the projection of collective many-body eigenmodes onto the motion of a tagged-particle. We are interested in the ‘confining’ (all background particles in front of the tagged-particle) and ‘pushing’ (all background particles behind the tagged-particle) scenarios for which we find non-trivial and qualitatively different relaxation behavior. Notably and somewhat unexpectedly, at fixed particle number we find that the higher the barrier the more prominent are the signatures of memory. Our results can readily be tested experimentally and may be relevant for understanding transport in biological ion-channels.

I. INTRODUCTION

Non-linear stochastic flows are at the heart of thermally driven processes in systems whose potential energy surfaces are characterized by multiple local energy minima. Pioneered by the seminal work of Kramers\cite{Kramers1940}, the concept of thermally activated barrier-crossing has ever since been applied to diverse phenomena, incl. chemical reactions\cite{Bell2013}, tunnel-diodes\cite{Bauer2005}, laser-pumping\cite{Blaauw2004}, magnetic resonance\cite{vanHaarlem2010b}, conformational dynamics and folding of proteins\cite{Oberhauser2008,Seifert2018} and nucleic acids\cite{Methfessel2002} and receptor-ligand binding\cite{van Kampen1992} to name but a few.

From a theoretical point of view, the most detailed and precise results were obtained in the context of relaxation phenomena\cite{Risken1984,Seifert2010} and first passage time statistics\cite{Kramers1940,Seifert2010} in Markovian (i.e. memory-less) systems. However, physical observables typically correspond to lower-dimensional projections and the observed dynamics is Markovian only under quite restrictive conditions on the nature of the projection\cite{van Kampen1992}. Quoting van Kampen: "Non-Markov is the rule, Markov is the exception"\cite{van Kampen1992}.

Over the years non-Markovian barrier crossing has therefore received special attention. Most approaches considered a generalized Langevin equation in the underdamped regime with diverse phenomenological memory kernels for the velocity in the high\cite{van Kampen1992,Seifert2010} and low\cite{Risken1984} viscosity limit. In the case of diffusion in double-well potentials unified solutions have been obtained\cite{Risken1984}. Seminal results on non-Markovian effects in the crossing of high energy barriers have been obtained by Mel’nikov and Meshkov\cite{Mel'nikov1984} and were later extended to low barriers by Kalmykov, Coffey and Tolstov\cite{Kalmykov2007}. Important results on non-Markovian barrier-crossing have been obtained in the context of condensational physics\cite{Kalmykov2007} and the role of hydrodynamic memory in surmounting energy barriers\cite{Seifert2010}. More recent studies of memory effects in bi-stable potentials have been carried out in the context of conformational dynamics of macromolecules\cite{Seifert2010} and the role of hydrodynamic memory in surmounting energy barriers\cite{Seifert2010}. While recent applications involve the interpretation of experiments on the folding of a DNA hairpin\cite{Blaauw2005}.

Quite detailed analytical results have also been obtained for overdamped non-Markovian stochastic flows in bi-stable potentials, in particular for exponentially correlated noise\cite{Chernyak2004,Chernyak2005,Chernyak2006}. Characteristic of these studies is that the memory is introduced phenomenologically and/or the systems typically possess slow and fast degrees of freedom. Thereby, integrating out of fast degrees of freedom leads to memory, and time-scales similar to, or longer than, the correlation time are of interest.

Here, we are interested in the scenario where the background degrees of freedom (i.e. those that become integrated out) relax on exactly the same time scale as the observable. In particular, we are interested in the relaxation dynamics of a tagged-particle in a single-file of Brownian particles confined to a bi-stable potential, and investigate the rôle of the height of the potential barrier. Projecting out particles’ positions introduces memory and strongly breaks Markovianity\cite{van Kampen1992}. The more particles’ coordinates become integrated out the stronger Markovianity is broken\cite{van Kampen1992}. A distinguishing characteristic of our approach with respect to the existing literature is, therefore, that we do not introduce memory phenomenologically via a generalized Langevin equation. Instead, the memory arises explicitly as a result of projecting out degrees of freedom in an exactly solvable Markovian many-body system.

Single-file models are generically used to describe strongly correlated, effectively one-dimensional, systems and processes, e.g. biological channel\cite{Blaauw2005}, transport in zeolites\cite{Chernyak2004}, crowding effects in gene regulation\cite{Suter2001}, superionic conductors\cite{Methfessel2002}, and strongly correlated one-dimensional soft matter systems in general\cite{Seifert2018}. Over the past years diverse theoretical studies yielded deep insight about the anomalous tagged-particle diffusion\cite{Seifert2018} and the emergence and meaning of memory\cite{Seifert2018}. Single-file diffusion in potential landscapes has been studied by computer simulation\cite{van Kampen1992}. However, the rôle of crowding/steric obstruction and particle correlations in barrier-crossing, and in particular in the relaxation towards equilibrium, has so far remained elusive.

In this work we provide in Sec. [II] an analytical solution to the problem using the coordinate Bethe ansatz. In Sec. [III] we analyze the equilibrium correlation time as a function of the barrier height and number of particles in the single-file. Sec. [IV] addresses the relaxation to equilibrium from a fixed,
non-equilibrium initial condition of the tagged-particle in the ‘confining’ and ‘pushing’ scenario, respectively. We conclude with a brief discussion incl. potential applications and extensions of our results.

II. THEORY

We consider a single-file of \( N \) point-particles confined to a box of length \( L = 2\pi \). In the center of the box there is a square-top energy barrier of width \( \pi \) and height \( U_b \) (see Fig. 1b). More precisely, each particle experiences the potential

\[
U(x) = \begin{cases} 
0, & \pi > |x| > \pi/2 \\
U_b, & |x| \leq \pi/2 \\
\infty, & \text{otherwise}.
\end{cases}
\]

(1)

The particles move according to overdamped Brownian dynamics under non-crossing conditions. For simplicity and without loss of generality we set \( D = 1 \), which is equivalent to expressing time in units of \( 4\pi^2/D \), and express \( U \) in units of thermal energy \( k_b T \), i.e. \( U \rightarrow U/k_b T \). The probability density of the set of positions \( \{x_i\} = x \) of the \( N \) particles evolves according to the many-body Fokker-Planck equation

\[
\left( \partial_t - \sum_{i=1}^{N} \left[ \partial^2_{x_i} + \partial_{x_i} \{ \partial_{x_i} U(x_i) \} \right] \right) G(x,t|x_0) = 0,
\]

(2)

with initial condition \( G(x,0|x_0) = \prod_{i=1}^{N} \delta(x_i - x_{0i}) \) and where the operator in curly brackets \( \{ \} \) acts only within the bracket. Eq. (2) is equipped with the set of external and internal boundary conditions

\[
\partial_{x_i} G(x,t|x_0)|_{x_i=-\pi} = \partial_{x_i} G(x,t|x_0)|_{x_i=\pi} = 0, \\
(\partial_{x_{i+1}} - \partial_{x_i}) G(x,t|x_0)|_{x_{i+1}=x_i} = 0,
\]

(3)

and is solved exactly using the coordinate Bethe ansatz (for technical details refer to Refs. [35, 71] and [75]). The resulting many-body Green’s function reads

\[
G(x,t|x_0) = \sum_{k} \Psi_R^k(x_0) \Psi_L^k(x_0) e^{-\lambda_k t},
\]

(4)

where \( \Psi_L^k(x) \) and \( \Psi_R^k(x) \) are the so-called left and right Bethe eigenfunctions, respectively, defined as

\[
\Psi_L^k(x) \equiv \mathcal{N}^{1/2} \partial_x \sum_{\{i\}} \prod_{i=1}^{N} \Psi_{L,i}^k(x_i),
\]

(5)

where \( \Psi_{L,i}^k(x) \) are the orthonormal eigenfunctions of the single-particle problem (given in Appendix), the sum over \( \{k\} \) refers to the sum over all permutations of the multiset \( k \), and \( \mathcal{N} \) is the number of these permutations. \( \lambda_k = \sum_{i=1}^{N} \lambda_{k,i} \) refers to the Bethe eigenvalue with multi-index \( k = \{k_i\}, i \in [1, N] \), and \( \partial_x \) is the particle-ordering operator, which ensures that \( x_1 \leq \cdots \leq x_i \leq \cdots \leq x_N \). Moreover, \( \lambda_n \) refer to the eigenvalues of the respective one-body problem given by

\[
\lambda_n = \begin{cases} 
\frac{n^2}{4}, & \text{mod}(n,4) = 0, \\
\left( \frac{n-1}{2} + \nu \right)^2, & \text{mod}(n,4) = 1, \\
\frac{n^2}{4}, & \text{mod}(n,4) = 2, \\
\left( \frac{n+1}{2} - \nu \right)^2, & \text{mod}(n,4) = 3
\end{cases}
\]

(6)

where \( \nu = 2 \arctan(e^{-U_b/2})/\pi \) and mod \((k,l)\) stands for the remainder of the division \( k/l \).

We are interested in the non-Markovian probability density of \( x_i \), the position of the \( i \)-th tagged-particle under the condition that the initial positions of the remaining particles are drawn from those equilibrium configurations that contain particle \( i \) at \( x_0 \), which reads (for a derivation see [35, 71] and [75])

\[
\mathcal{G}(x_i,t|x_{0i}) = V_{00}^{-1}(x_{0i}) \sum_{k} V_{0k}(x_i) V_{k0}(x_{0i}) e^{-\lambda_k t},
\]

(7)

where the ‘overlap-elements’ \( V_{kl}(x_i) \) are defined as

\[
V_{kl}(x_i) = \frac{m_l}{N_l!N_R!} \sum_{\{k\}} \prod_{i=1}^{N} \Psi_{L,i}^k(x_i) \prod_{m=i+1}^{N_l} \lambda_m(x_i) \prod_{m=i+1}^{N_R} R_m(x_i)
\]

(8)

with \( m_l \) being the multiplicity of the multiset \( I \), and \( N_l = i-1 \) and \( N_R = N-i \) are, respectively, the number of particles to the left and right of the tagged-particle. In Eq. (8) we introduced the auxiliary functions

\[
L_n(x) = \int_{-\pi}^{\pi} dz \Psi_{n}^{L}(z) \Psi_{n}^{L}(z), \quad R_n(x) = \int_{-\pi}^{\pi} dz \Psi_{n}^{R}(z) \Psi_{n}^{R}(z).
\]

(9)

Note that the equilibrium probability density of the tagged-particle’s position is given by (see Eq. (7))

\[
\mathcal{G}_{eq}(x_i)(x_{0i}) \equiv \lim_{\tau \rightarrow \infty} \mathcal{G}(x_i,t|x_{0i}) = V_{00}^{-1}(x_i)
\]

and is depicted for various values of \( U_b \) in Fig. 1b-d. Intuitively, as \( U_b \) increases particles become expelled from the barrier.

In Ref. [75] we have developed an algorithm designed to efficiently cope with the combinatorial complexity of the implementation of the analytical solution in Eq. (7). Due to the piece-wise constant nature of the potential \( U(x) \) in Eq. (1) all integrals (9) can be computed analytically. As the resulting expressions are lengthy we do not show them here. Instead, they are readily implemented in an extension of the code published in Ref. [75] (see Supplementary Material).

III. LINEAR CORRELATIONS AT EQUILIBRIUM

First we consider linear correlations at equilibrium and limit the discussion in the reminder of the paper to tagging the first or last particle (i.e. throughout we set \( i = 1 \) or \( i = N \)).
That is, we are interested in the normalized positional auto-
correlation function of a tagged-particle defined as

$$C_i(t) = \frac{\langle x_i(t) x_i(0) \rangle - \langle x_i \rangle^2}{\langle x_i^2 \rangle - \langle x_i \rangle^2},$$

where the covariance of the position is defined as

$$\langle x_i(t) x_i(0) \rangle = \frac{\pi}{2} \int_{-\pi}^{\pi} dx_i \int_{-\pi}^{\pi} dx_{i0} x_i x_{i0} \mathcal{P}_{eq}(x_i) \mathcal{P}_{eq}(x_{i0}),$$

and $\langle x_i^2 \rangle = \frac{\pi}{2} \int_{-\pi}^{\pi} dx_i x_i^2 \mathcal{P}_{eq}(x_i)$. The above integrals have been performed numerically by means of Gauss-Kronrod quadrature. Note that Eq. (10) alongside Eqs. (5-9) necessarily implies the structure $C_i(t) = \sum_k a_k e^{-\Lambda_k t}$ with $\sum_k a_k = 1$ and where all $a_k \geq 0$. The results for $C_i(t)$ as a function of the barrier height $U_b$ are depicted in Fig. 2. Since $U(x)$ is symmetric, the autocorrelation functions of the first and last particle coincide, i.e. $C_1(t) = C_N(t)$.

The autocorrelation of an isolated particle (i.e. $N = 1$) in Fig. 2a displays for a given value of $U_b$ to a good approximation an exponential decay with rate $\Lambda_1 = \Lambda_1$ given by Eq. (5). This reflects that positional correlations decay predominantly due to barrier-crossing. Conversely, as the number of particles increases $C_i(t)$ decays on multiple time-scales (see Fig. 2b) and develops an “anomalous” shoulder on shorter time-scales,37,38,39 which span increases with the barrier height $U_b$. A comparison of $C_i(\Lambda_1^{-1})$ reveals that the relative decay of correlations from the relaxation time $\tau_{rel} \equiv \Lambda_1^{-1}$ onward is substantially reduced for about a factor of 2 compared to the isolated particle case. $\tau_{rel}$ denotes the time-scale on which the system reaches equilibrium from any initial condition. Note that (i) $C_1(t)$ measures relative correlations and (ii) according to Eq. (7) terminal relaxation roughly corresponds to the particles individually crossing the barrier several times. It is also important to note that the natural time-scale of a tagged-particle is set by the average collision time $\tau_{col} = 1/N^2$ which decreases with increasing $N$. That is, in units of the average number of collisions $t \to t/\tau_{col}$ correlations decay more slowly for larger $N$.

A common means to quantify the extent of correlations found in the literature is the so-called correlation time $\tau_{col}$ that (i) measures relative correlations and (ii) according to Eq. (7) terminal relaxation roughly corresponds to the particles individually crossing the barrier several times. It is also important to note that the natural time-scale of a tagged-particle is set by the average collision time $\tau_{col} = 1/N^2$ which decreases with increasing $N$. That is, in units of the average number of collisions $t \to t/\tau_{col}$ correlations decay more slowly for larger $N$.

$$T_c = \int_0^\infty dt C_i(t), \quad \tau_{col} \equiv \Lambda_1^{-1} = \left( \frac{2}{\pi} \arctan(e^{-U_b/2}) \right)^{-2},$$

where we note that for high barriers, i.e. $U_B \gg 1$, the relaxation time follows the expected Arrhenius scaling $\tau_{col} \approx 4e^{U_b/2}$. In Fig. 3a we depict the correlation time for the leftmost particle in units of $\tau_{col}$ as a function of the barrier height $U_b$ for different $N$. For an isolated particle $T_c = T_c^{isolated}$ agrees very well with $\tau_{col}$ for all values of $U_b$, confirming the idea that $C_i(t)$ decays to a very good approximation as a single exponential. Note that, for systems obeying detailed balance, the mathematical structure of $C_i(t)$ trivially implies a shorter correlation time as soon as $C_i(t)$ decays on multiple time-scales if the longest time-scale $\Lambda_1^{-1}$ is the same. This is particularly true when comparing $C_i(t)$ of a tagged-particle in a single-file with an isolated particle. Namely,

$$T_c = \sum_k a_k/\Lambda_k \leq \sum_k a_k/\Lambda_1 = \Lambda_1^{-1} \approx T_c^{isolated}. \quad (13)$$

Therefore, the interpretation of $T_c$ should always be made cautiously and in the particular case of tagged-particle diffusion in a single-file is not meaningful if we consider $T_c$ on an absolute scale. However, it becomes somewhat more meaningful on the natural time-scale, i.e. when time is expressed in terms of the natural number of inter-particle collisions (see also35). Inspecting $C_i(t)$ on this natural time scale we find in Fig. 3b that the tagged-particle on average undergoes more collisions before it decorrelates for larger values of $N$, and this number increases with increasing $U_b$.

Moreover, as $N$ increases the space explored by a tagged-particle becomes progressively more confined rendering the correlation time $T_c$ on an absolute time-scale also intuitively
shorter. Indeed, in Fig. 3b we depict the ratio $T_c/\Lambda_1^{-1}$ which decreases with increasing $N$ for any barrier height $U_b$. Note that $\Lambda_1^{-1}$ is independent of $N$ and the breaking of Markovianity (reflected, e.g. in the violation of the Chapman-Kolmogorov semi-group property[55]) is encoded entirely in the overlap elements $V_{0k}, V_{k0}$. For systems with microscopically reversible dynamics $T_c/\Lambda_1^{-1} < 1$ quite generally implies that relaxation evolves on multiple time-scales. Thus, the results in Fig. 3b suggest, in agreement with intuition, that more and more time-scales are involved in the relaxation of a tagged-particle’s position in equilibrium as we increase $N$. In other words, on the level of linear correlations signatures of memory of the initial conditions of ‘latent’/background particles are reflected in the multi-scale relaxation of $C_1(t)$.

IV. RELAXATION FROM A PINNED CONFIGURATION

We now focus on the ‘complete’ (i.e incl. correlations to all orders) relaxation to equilibrium from a pinned configuration. That is, we are interested in those initial configurations where either the first ($i = 1$) or the last ($i = N$) particle is pinned at $x_0$, while the initial conditions of the remaining particles are drawn from the corresponding pinned equilibrium (i.e. those equilibrium many-body configurations where the first/last particle is located at $x_0$).

We quantify the relaxation dynamics by means of $\mathcal{D}(t,x_0)$, the Kullback-Leibler divergence[80] between the non-Markovian probability density of the tagged-particle’s position at time $t$, $\mathcal{D}(x,t|x_0)$ in Eq. 7, and the respective equilibrium density $\mathcal{P}_{eq}(x_i) \equiv \lim_{t \to +\infty} \mathcal{D}(x_i,t|x_0)$:

$$\mathcal{D}(t,x_0) \equiv \int_{-\infty}^{\infty} dx \mathcal{D}(x,t|x_0) \ln \left( \frac{\mathcal{P}(x,t|x_0)}{\mathcal{P}_{eq}(x)} \right).$$

(14)

In physical terms $\mathcal{D}(t,x_0)$ represents the displacement from equilibrium in the sense of an excess instantaneous free energy, i.e. $k_B T \mathcal{D}(t,x_0) = F(t) - F[18][53]$ Since the integral in Eq. (14) cannot be performed analytically we evaluate it numerically. We always pin the initial position of the tagged-particle at $x_0 = -2$. According to the effect of the pinning on the relaxation of the tagged-particle, the scenario in which we tag the first particle is referred to as ‘confining’ (since background particles obstruct the relaxation of the tagged-particle) and the one in which we tag the first particle as ‘pushing’ (since background particles exert an entropic force pushing the tagged-particle over the barrier). $\mathcal{D}(t,x_0)$ as a function of the barrier height $U_b$ for $N = 5$ and $N = 9$ is shown in Fig. 4.

Note that $\lim_{t \to +\infty} \mathcal{D}(t,x_0) = 0$ irrespective of $N$ and $U_b$ since we are comparing a delta distribution with a smooth probability density. Conversely, in an arbitrarily small time interval $\tau > 0$ the non-Markovian tagged-particle density $\mathcal{D}(x,t|x_0)$ evolves to a smooth, well-behaved probability density such that $\mathcal{D}(t > 0,x_0)$ is always finite and the ‘pathology’ at $t = 0$ is mathematical and not physical.

With this in mind we observe in Fig. 4 a striking difference between the ‘confining’ and ‘pushing’ scenario. In the ‘confining’ setting $\mathcal{D}(t,x_0)$ at a fixed time $t$ is a monotonically increasing function of $U_b$ and as a function of time decays on a time-scale that seems to be rather independent of $U_b$. In the ‘confining’ scenario an increase of $U_b$ displaces the system at $t = 0^+$ further from equilibrium. This is intuitive because $\mathcal{P}_{eq}(x_i)$ becomes more strongly confined to the boundary and hence away from $x_0$. To a dominant extent relaxation occurs already on time-scales $t \gtrsim 1 \ll \Lambda_1^{-1}$. The reason may be found in the fact that $\Lambda_1^{-1}$ corresponds to the mixing/ergodic time-scale on which the full single-file (and thus the tagged-particle) explores the entire system. In the ‘confining’ scenario the background particles are drawn from a distribution that resembles closely the unconstrained equilibrium and, in addition, the tagged-particle is nominally unlikely to be found in the right well in equilibrium. Therefore, the fraction of paths that cross the barrier in the ensemble of relaxation paths is small, rendering $V_{0k} V_{k0}$ for low-lying $k$ essentially negligible (see Eq. 7). Nevertheless, a second, slower relaxation stage is still discernible at $t \gtrsim 1$.

Conversely, in the ‘pushing’ scenario depicted in Fig. 4 and [44] we find (i) the dependence of $\mathcal{D}(0^+,x_0)$ on $U_b$ to be inverted, and (ii) for given $N$ and $U_b$ relaxation extends
to much longer time-scales compared to the 'confining' scenario. In order to rationalize (i) we consider a pair of barriers $U_{b1}, U_{b2}$ and take the limit

$$\lim_{t \to 0} \left( \mathcal{D}^{b_1}(t, x_0) - \mathcal{D}^{b_2}(t, x_0) \right) = \ln \left( \mathcal{D}^{b_2}_{\text{eq}}(x_0) / \mathcal{D}^{b_1}_{\text{eq}}(x_0) \right),$$

(15)

which is finite and well defined despite the fact that $\lim_{t \to 0} \mathcal{D}^{b_1, b_2}(t, x_0)$ are infinite. Eq. (15) explains that the dependence of $\mathcal{D}(0^+, x_0)$ on $U_b$ is not unique and depends on the pinning point $x_0$ which determines whether or not $\mathcal{D}^{b}_{\text{eq}}(x_0) / \mathcal{D}^{b}_{\text{eq}}(x_0)$ is greater or smaller than 1 (see Fig. 1b and [4]). (ii) can be understood by an extension of the argument put forward in the discussion of the 'confining' scenario, i.e., as a result of the pinning the initial configurations of the background particles are displaced much further away from equilibrium, rendering $\nu_{\text{b,k}}\nu_{\text{b,k}}$ for low-lying $k$ substantial (see Eq. (7)). Therefore, a pronounced second relaxation stage is visible at longer times $t \gtrsim 1$.

Based on Fig. 4 alone we are not able to deduce whether these observations are a trivial consequence of the pinning in the sense that they have nothing to do with memory (note that a Markov process 'remembers' the initial condition up to $\sim \tau_0$) or whether they are in fact a signature of memory in the dynamics. Additional insight is gained by inspecting the relaxation of the full, Markovian single-file evolving from the same initial condition, i.e.,

$$\mathcal{D}_M(t, x_0) \equiv \frac{N}{\pi} \int_{-\pi}^{\pi} dx_i \, G(x, t, R_i) \ln \left( \frac{G(x, t, R_i)}{P_{\text{eq}}(x)} \right),$$

(16)

were we have introduced the joint Markovian two-point probability density $G(x, t, R_i) \equiv \int dy_0 G(x, t, y_0) P_0(y_0)$ whereby, for $-\pi < x_0 < -\pi/2$, $P_0(y)$ is defined as

$$P_0(y) = N! (\pi + x_0)^{-N} \cdot \delta(x_0 - y) \cdot e^{-U_b \sum_{j=1}^{N} \theta(\pi/2 - |x_j|)} / (\pi e^{U_b - x_0} N^N),$$

(17)

where $\theta(x)$ is the Heaviside step function, and $P_{\text{eq}}(x) = \lim_{t \to \infty} G(x, t, x_0)$. The integration in Eq. (16) can be performed analytically (for details please see Ref. [33]). Introducing the two-point joint density of the single-particle problem

$$\Gamma_i(x, a, b) \equiv \sum_{x'} \psi_{j}(x') \int_{-\pi}^{\pi} dy \psi_{i}(y) P_0(y) e^{-U(y)} \text{ with } P_0(y) \equiv \theta(-\pi/2 - y)/(\pi + x_0 + \theta(y + \pi/2) e^{-U(y)}/(\pi e^{U_b - x_0})$$

as well as the auxiliary function

$$\Xi_i(a, b) \equiv \int_{-\pi}^{\pi} dx_i \Gamma_i(x, a, b) / (\pi e^{U_b - x_0}) \text{ with } P_0(x) = e^{-U(x)}/(\pi(1 + e^{-U_b})},$$

(18)

where $P_{\text{eq}}(x) = e^{-U(x)}/(\pi(1 + e^{-U_b}))$, the result reads

$$\mathcal{D}_M(t, x_0) = \Xi_i(-\pi, x_0) \Xi_i(-\pi, x_0)^N \Xi_i(x_0, \pi)^N.$$

(19)

An explicit solution is obtained with the aid of Mathematics. As it is bulky but straightforward we do not show it here. The Markovian result in Eq. (19) for the same set of parameters as in Fig. 4b and 5b is depicted in Fig. 5. A comparison of Figs. 4 and 5 reveals that the second, long-time relaxation stage observed in the 'pushing' scenario in Fig. 4 is absent in the Markovian setting (compare Figs. 4a and 5) and note that the relaxation time $\Lambda^{-1}$ is identical in both settings). This in turn implies that the pronounced second relaxation stage in the non-Markovian, tagged-particle scenario at times $t \gtrsim 1$ is indeed a signature of memory.

V. DISCUSSION

We identified pronounced signatures of memory in the overdamped relaxation of a tagged-particle in a single-file confined to a bi-stable potential. On the level of linear correlations in equilibrium memory is visible in the form of a multi-scale relaxation of the autocorrelation function (see Fig. 2) and a seemingly paradoxical shortening of the so-called correlation time $T_c$ (see Fig. 3). The latter was shown to be an artifact of the definition of $T_c$. When including the complete correlation-structure as encoded in the so-called excess instantaneous free energy (see Eq. (14)) distinctive signatures of memory emerge in the form of a second, late-time relaxation regime.

The memory originates from the fact that the entire single-file relaxes to equilibrium in the form of linearly independent many-body eigenmodes, which become projected on the motion of a tagged particle. The projection couples distinct modes thus braking Markovianity and giving rise to memory. It turns out to be very important which particle is tagged. Here, we were only interested in the 'confining' (all background particles in front of the tagged particle) and 'pushing' (all background particles behind the tagged particle) scenarios and found qualitatively different relaxation behavior. A systematic analysis would be required to understand the intricate details in how the number of particles on each side affects relaxation dynamics, which is beyond the scope of this Communication.

Our results can readily be tested by existing experiments probing colloidal particle systems (see e.g. [34,37], and may furthermore be relevant for a theoretical description of transport in ion-channels [39,40]. Our results can be extended in diverse ways, most immediately by including other types of inter-particle interactions [42] and time-dependent energy barriers [43].
VI. APPENDIX

In this Appendix we give explicit expressions for the single-particle eigenfunctions that are required in the diagonalization of the many-body Fokker-Planck operator using the so-called coordinate Bethe ansatz. For details of the solution method please see \cite{35,71}. The eigenfunctions of the corresponding single-particle eigenvalue problem

\[
\begin{align*}
(\partial_x^2 + \partial_x \{ \partial_x U(x) \} ) \psi_k^R(x) &= -\lambda_k \psi_k^R(x) \\
(\partial_x^2 - \{ \partial_x U(x) \} \partial_x) \psi_k^L(x) &= -\lambda_k \psi_k^L(x),
\end{align*}
\]  

where \( \psi_k^L,R(x) : [-\pi, \pi] \to \mathbb{R} \) allow for a spectral decomposition of the single-particle Green’s function

\[ \Gamma(x,t|x_0) = \sum_k \psi_k^R(x) \psi_k^L(x_0) e^{-\lambda_k t}. \]  

(21)

\( \psi_k^L,R(x) \) enter Eq. (5) and are here defined via their ‘Hermitianized’ counterpart \( \psi_k(x) : [-\pi, \pi] \to \mathbb{R} \) as \( \psi_k^R(x) = e^{-U(x)/2} \psi_k(x), \psi_k^L(x) = e^{U(x)/2} \psi_k(x) \) where \( \psi_k(x) = \sqrt{\frac{2}{1 + \delta_{k,0}}} e^{-U(x)/2} \cos(\sqrt{\lambda_k} x), \mod(k, 4) = 0 \) \[ 22 \]

\[
\psi_k(x) = \begin{cases} 
\cos(\sqrt{\lambda_k}(x + \pi)) \sqrt{\pi} , & x < -\pi/2 \\
\sin(\sqrt{\lambda_k} x) \sqrt{\pi} , & |x| \leq \pi/2 , \mod(k, 4) = 1 \\
\cos(\sqrt{\lambda_k}(x - \pi)) \sqrt{\pi} , & x > \pi/2
\end{cases}
\]  

(23)

\[
\psi_k(x) = \sqrt{\frac{2}{1 + \delta_{k,0}}} e^{-U(x)/2} \cos(\sqrt{\lambda_k} x), \mod(k, 4) = 2
\]

\[
\psi_k(x) = \begin{cases} 
\cos(\sqrt{\lambda_k}(x + \pi)) \sqrt{\pi} , & x < -\pi/2 \\
\sin(\sqrt{\lambda_k} x) \sqrt{\pi} , & |x| \leq \pi/2 , \mod(k, 4) = 3, \\
\cos(\sqrt{\lambda_k}(x - \pi)) \sqrt{\pi} , & x > \pi/2
\end{cases}
\]  

(24)

where \( \delta_{k,0} \) is the Kronecker delta.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request. An extension of the code published in Ref. \cite{79} that implements the analytical results presented this manuscript is included in the Supplementary Material.

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82 We here correct typos found in the original publications.