Efficient numerical solver for time-dependent Fokker–Planck equations

Viktor Holubec,1,2 Klaus Kroy,1 and Stefano Steffenoni1,3

1Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany
2Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, V Holešovičkách 2, CZ-180 00 Praha, Czech Republic
3Max Planck Institute for Mathematics in the Sciences, Inselstr. 22, D-04103 Leipzig, Germany

(Dated: April 5, 2018)

We present a simple but powerful method for solving time-dependent Fokker–Planck equations (FPE) for over-damped stochastic processes, also known as Smoluchowski equations. It yields both transition and steady-state behavior and allows for efficient computations of moment-generating and large-deviation functions of observables defined along stochastic trajectories, such as the fluctuating work and heat. The method is based on a direct computation of the time-ordered exponential representing the propagator of the FPE, discretized in space and time. To test the performance of the method and to exemplify its potential for applications, we compare it against Brownian-dynamics simulations of an active Brownian particle trapped in a time-dependent quartic potential.

I. INTRODUCTION

Many natural phenomena exhibit a scale separation between “slow” and “fast” degrees of freedom. The variables varying slowly in space or time can then be characterized by a self-contained coarse-grained dynamics, which is — for not too large systems — perceptibly perturbed by fluctuations arising from the noisy dynamics of the fast variables. The flourishing field of stochastic thermodynamics provides a general framework to deal with these fluctuating coarse-grained degrees of freedom of microscopic objects such as Brownian particles, individual proteins, or living bacteria, which often operate under conditions far from equilibrium [1, 2].

The Fokker–Planck equation (FPE) represents a most comprehensive description of such time-separated phenomena. It predicts not only the average dynamics of the remaining fast variables but directly addresses, in a technically manageable way, their complete probability distribution, which includes the complete information about the fluctuations induced by the fast degrees of freedom. To achieve this, all of the slow variables need to be resolved explicitly in a so-called Markovian description, such that the remaining fast variables evolve without perceptible memory of the past dynamics. Over the last century, the FPE found applications in various scientific disciplines ranging from physics and chemistry to biology and ecology and even economy and finance [4–10]. Needless to say that it can only in very few special cases be solved analytically, so that one usually has to resort to analytical approximations, computer simulations and numerical methods [4, 11–13]. Both the Fokker–Planck formulation of stochastic dynamics and efficient numerical solution have become particularly relevant for situations far from equilibrium, where the slow variables are, as a rule, found to exhibit unconventional characteristic fluctuations that contain a crucial part of the interesting information about the system of interest.

In the following, we report a simple but efficient matrix numerical method (MNM) for solving over-damped FPEs with time-dependent coefficients, also known as Smoluchowski equations. The method is widely applicable to various types of functionals used to describe the fluctuations of observables defined along the trajectories of the corresponding stochastic process, such as their characteristic functions (CHFs), moment generating-functions (MGFs) and large-deviation functions (LDFs), for example. The MNM can address all of these functions directly. It is based on a direct discretization of space and time that allows to calculate the Green function of the FPE from the time-ordered exponential representation of the discretized propagator.

We test and illustrate the power of the MNM by focusing on a specific example, namely an over-damped active particle trapped in a time-dependent quartic potential and communicating with a bath with time-dependent temperature. We investigate the unconventional Brownian dynamics of the particle and the fluctuations of work and heat exchanged with the bath, using both the proposed MNM and Brownian dynamics simulations (BD). While both approaches give the same results, the MNM is often much faster than the BD.

II. MATRIX NUMERICAL METHOD

For pedagogical reasons, we introduce the MNM for a two-dimensional stochastic system, parametrized by the “spatial” and “angular” coordinates $x$ and $\theta$, respectively. An extension to higher dimensions is straightforward. The FPE reads

$$\partial_t \rho = [D_x \partial_{xx} + D_\theta \partial_{\theta\theta} + \mu_x \partial_x (\partial_x U_x) + \mu_\theta \partial_\theta (\partial_\theta U_\theta)] \rho$$

(1)

with time-dependent coefficients. The “angular” potential $U_\theta$ is defined on the compact domains $\theta \mod 2\pi$. Similarly, we require that the “spatial” potential $U_x$ obeys the confinement condition $\lim_{x \to \infty} U_x(\pm x, \theta, t) = \ldots$
infinity, which allows it to be effectively redefined as a potential with finite support (by setting $U_x(x,\theta, t) = \infty$ for all $|x| > x_\infty$), without affecting the resulting dynamics of the system. Otherwise, we allow for arbitrary time-independent $U_x$ and $U_\theta \neq U_x$ (both in general dependent on $x$ and $\theta$ in different ways), which includes the possibility of non-conservative forces, and for different temperatures $D_x/\mu_x \neq D_\theta/\mu_\theta$ of the two degrees of freedom. Apart from the limitation of bounded (possibly periodic) domains, which can be relaxed with some extra effort \cite{Gray}, Eq. \eqref{eq:1} thus provides us with a completely general description of over-damped stochastic dynamics. In particular, even the stationary solution, obeying $\partial_t \rho = 0$, will in general be a non-equilibrium one, which usually cannot be determined analytically \cite{Gray}, let alone the fully time-dependent solution.

The main idea to solve the complicated time-dependent equation \eqref{eq:1} is to first integrate it incrementally for constant coefficients. Then one uses the Markov property of the compound stochastic process $(x, \theta)$ to construct a step-wise approximation to the full Green function. By adapting the discretization mesh to the salient features of the time-dependent driving, one can thus strike a good balance between accuracy and efficiency. For the first step of this program, we follow Refs. \cite{Gray,Gray} and discretize the two-dimensional continuous state-space $(x, \theta)$ into $(N_x+1)(N_\theta+1)$ discrete state points with coordinates $(i_x, i_\theta)$,

\begin{align}
    i_x &= \lfloor (x + x_\infty)/\Delta_x \rfloor, \quad \Delta_x = 2x_\infty/N_x, \quad (2) \\
    i_\theta &= \lfloor (\theta \mod 2\pi)/\Delta_\theta \rfloor, \quad \Delta_\theta = 2\pi/N_\theta, \quad (3)
\end{align}

as illustrated in Fig. \ref{fig:1}. This crucially exploits the compact support of the solution $\rho(x, \theta, t)$. The diffusion in continuous state-space is then approximated by a jump process on this discrete lattice. Only transitions between the neighboring lattice points are allowed (c.f. the arrows in Fig. \ref{fig:1}). With transition rates given by

\begin{align}
    r_{i_x,i_\theta \rightarrow i_x \pm 1,i_\theta} &= \frac{D_x}{\Delta_x} e^{-\frac{2\pi\theta}{\Delta_\theta}[V_x(i_x \pm 1,i_\theta)\mp V_x(i_x,i_\theta)]}, \\
    r_{i_x,i_\theta \rightarrow i_x,i_\theta \pm 1} &= \frac{D_\theta}{\Delta_\theta} e^{-\frac{\pi \theta}{\Delta_\theta}[V_\theta(i_x,i_\theta \pm 1)\mp V_\theta(i_x,i_\theta)]}.
\end{align}

Note that the upper index is fixed during the jump described by the lower index, and that we introduced the shorthand notation $V_x(i_x, i_\theta) \equiv U_x(-x_\infty + \Delta_x i_x, \Delta_\theta i_\theta)$, $V_\theta(i_x, i_\theta) \equiv U_\theta(-x_\infty + \Delta_x i_x, \Delta_\theta i_\theta)$. With these transition rates, the dynamics of the occupation probabilities $p_{i_x,i_\theta}(t)$ of the individual lattice points $i_x, i_\theta$ is governed by the Master equation \eqref{eq:19}

\begin{align}
    \dot{p}_{i_x,i_\theta} &= r_{i_x,i_\theta+1,i_\theta+1} p_{i_x+1,i_\theta+1} + r_{i_x+1,i_\theta,i_\theta} p_{i_x+1,i_\theta} + \\
    &- r_{i_x,i_\theta-1,i_\theta-1} p_{i_x-1,i_\theta-1} - r_{i_x-1,i_\theta+1,i_\theta} p_{i_x-1,i_\theta+1} - r_{i_x,i_\theta-1,i_\theta} p_{i_x,i_\theta-1},
\end{align}

which is equivalent to the FPE \eqref{eq:11} with constant coefficients, in the continuum limit $\Delta_x \rightarrow 0$, $\Delta_\theta \rightarrow 0$, as can be checked by direct calculation. The solution $\rho(x, \theta, t)$ of the partial differential equation \eqref{eq:11} can thus be calculated as

\begin{equation}
    \rho(x, \theta, t) = \lim_{\Delta_x \rightarrow 0} \lim_{\Delta_\theta \rightarrow 0} p_{i_x,i_\theta}(\theta(t)). \quad (7)
\end{equation}

An important feature of this discretization method is that the transition rates \eqref{eq:19} fulfill the condition

\begin{equation}
    e^{\frac{2\pi}{\Delta_\theta} V_\theta(i_x,i_\theta)} e^{\frac{\pi}{\Delta_\theta} V_\theta(i_x,i_\theta \pm 1)} = r_{i_x,i_\theta} e^{\frac{\pi}{\Delta_\theta} V_\theta(i_x,i_\theta \mp 1)} \quad (8)
\end{equation}

along the $x$-axis, which amounts to a “global” detailed balance in this coordinate \cite{Gray1}. A similar condition holds for the transition rates \eqref{eq:19} in the $\theta$-direction. The discrete model described by Eqs. \eqref{eq:19}–\eqref{eq:21} is thus thermodynamically consistent for arbitrary discretization parameters $\Delta_x$ and $\Delta_\theta$, which ensures that the proposed numerical method gives physically reasonable results regardless of the discretization step. Of course, each of the two detailed-balance conditions is trying to draw the system into the Boltzmann equilibrium corresponding to its own temperature and potential $(D_x/\mu_x, V_x$ and $D_\theta/\mu_\theta, V_\theta$, respectively). Globally, this competition leads to a non-equilibrium stationary state.

The Master equation \eqref{eq:19} can be rewritten as

\begin{equation}
    \dot{\mathbf{p}}(t) = \mathcal{R} \cdot \mathbf{p}(t), \quad (9)
\end{equation}

where the elements of the $(N_x+1)(N_\theta+1)$ dimensional vector $\mathbf{p}(t)$ are given by the occupation probabilities $p_{i_x,i_\theta}(t)$. Still considering the case of constant coefficients in the FPE, the $(N_x+1)(N_\theta+1) \times (N_x+1)(N_\theta+1)$ matrix $\mathcal{R}$ is constant and contains the transition rates \eqref{eq:19}–\eqref{eq:21} in such a way that Eqs. \eqref{eq:19} and \eqref{eq:21} are equivalent.

The Green function for Eq. \eqref{eq:19} is then formally given by the matrix exponential

\begin{equation}
    \mathcal{U}(t,t_0) = \exp[\mathcal{R}(t-t_0)]. \quad (10)
\end{equation}

Because only jumps between the neighboring sites are allowed (see Fig. \ref{fig:1}), the time-independent jump matrix $\mathcal{R}$ is sparse, and $\mathcal{U}(t,t_0)$ can be obtained using fast numerical procedures for sparse matrices.
The ability to calculate the jump propagator $\mathcal{U}(t, t_0)$ for fixed constant coefficients eventually allows us to obtain the Green function for Eq. (11) with arbitrary time-dependent coefficients. This leads us to the announced second step in the development of the MNM. Namely, we discretize the time interval $[0, t_p]$ during which the Green function of the general FPE should be calculated into $N_t$ time slices of the length $\Delta t = t_p/N_t$. We assume that the driving can be approximated by appropriate constants during all of these intervals and that it may change only step-wise from one interval to the next. In other words, we replace the actual protocol $f(t)$ by a piece-wise constant approximation $\tilde{f}(t) = f(\Delta t i_t)$, $i_t = \lfloor t/\Delta t \rfloor$. The propagators for the individual time-intervals, during which the driving is constant, can be obtained using the procedure described above. Denoting by $\mathcal{U}_i$ the propagator $\mathcal{U}(i\Delta t, (i-1)\Delta t)$ corresponding to the $i$th time-interval, we can then obtain the approximate Green function under continuous driving for arbitrary $t > 0$ as

$$\mathcal{U}(t, 0) = \lim_{\Delta t \to 0} \prod_{i=1}^{\lfloor t/\Delta t \rfloor} \mathcal{U}_i \, . \quad (11)$$

For $t = 0$, it reduces to the identity matrix.

There are several ways how to determine suitable discretization parameters $N_x$, $N_\theta$ and $N_t$ and the potential cut-off $x_\infty$ without knowing the exact solution. First, one can study how the obtained results change with increasing values of these numbers. Once the difference becomes small, a further refinement of the discretization is not necessary. A second way, pursued below, is to compare the numerical results with results obtained using Brownian dynamics (BD) simulations of the stochastic process described by the FPE (11).

One may argue that the proposed MNM is a brute force method which will require a tremendous amount of computational time. While the former is indeed true, the latter turns out to be overly pessimistic, as we demonstrate, for a specific example, in the next section. For this example, we also show how the method can be used for the direct computation of moment-generating functions (MGFs) and large-deviation functions (LDFs) for various observables defined along stochastic trajectories described by the FPE (11). An important advantage of the MNM is indeed that it is easily set up in a “customized” way, optimized for a specific observable of interest.

### III. EXAMPLE: DRIVEN ACTIVE PARTICLE

Consider an active particle self-propelling with a velocity of magnitude $v(t)\cos\theta(t)$ and driven by a time-dependent quartic potential

$$U(x, t) = k(t)x^4/4 \quad (12)$$

in the $x$-direction, as shown in Fig. 2. We assume that the particle motion is overdamped and thus its position $x(t)$ and orientation $\theta(t)$ obey the first-order Langevin equations

$$\dot{x} = -kx^3 + v \cos \theta + \sqrt{2D_x}\xi_x, \quad (13)$$

$$\dot{\theta} = \sqrt{2D_\theta}\xi_\theta. \quad (14)$$

Here, $\xi_x$ and $\xi_\theta$ denote independent, zero-mean unit-variance Gaussian white noises so that the system corresponds to Eq. (11) with $\mu_x U_x = U - vx \cos \theta, \mu_\theta U_\theta = 0$.

Such schematic models of active particles are often considered as idealized caricatures of artificial or biological micro-swimmers [21–23]. In fact, they have acquired the status of a major new paradigmatic toy model of non-equilibrium statistical mechanics. While currently most studies resort to simulations when analytical approximations cease to work [13], the MNM could in the future provide a welcome alternative approach. To illustrate its application to the above model, we consider a specific non-equilibrium situation that is of interest for its own sake. Namely, motivated by recent studies interpreting trapped Brownian particles as microscopic heat engines [2–14,24–26], we choose the potential stiffness $k(t)$, the active particle velocity $v(t)$, and the diffusion coefficients $D_x(t)$ and $D_\theta(t)$ to be 1-periodic functions with a common period, as depicted in Fig. 3. For the sake of simplicity, all physical quantities are represented in suitable natural units that render them dimensionless.

Using the MNM, it is straightforward to determine the matrix $\mathcal{U}(t, 0)$ in Eq. (11), which represents the approximate Green function for the FPE of the model, during one driving cycle. It is a time-periodic function, as a consequence of the periodicity of the driving. We employed the formulas $p_1 = \mathcal{U}(1, 0)p_0 = p_0$ and $p(t) = \mathcal{U}(t, 0)p_0$ and the relation (7) to compute approximations to the probability distribution $\rho(x, \theta, t)$ of the active particle during the limit cycle attained at late times. These were then used to numerically compute the averages $\langle x^2 \rangle$, $\langle x \cos \theta \rangle$ and $\langle x^4 \rangle$ as functions of time and the marginal distribution for position $\xi(x, t) = \int_0^{2\pi} d\theta \rho(x, \theta, t)$ at five time instants $t = 0, 1/4, 1/2, 3/4$ and 1, during the limit cycle. We also independently evaluated these quantities using a corresponding BD simulation. The comparisons of the averages and the marginal distributions are shown in Figs. 4a/b, respectively. The MNM results, depicted by full lines, perfectly overlap with those of the BD (symbols). For the chosen discretization parameters
(N_x = 51, N_θ = 21, N_t = 76 and x_∞ = 2.4), the numerical calculation was approximately 10 times faster than the BD (10^5 trajectories and the integration step 10^{-3}). But already for N_x = 31, N_θ = 15, N_t = 76 and x_∞ = 2.4 one obtains curves that are visually indistinguishable from those depicted in Fig. 4 in which the MNM is approximately 100 times faster than the BD.

IV. MOMENT GENERATING FUNCTIONS

As an alternative to the conventional approach, namely to first compute the distribution ρ(x, θ, t) and then use it to get averages, moments, and reduced distribution functions for x and θ, the MNM also can advantageously directly be applied to other comprehensive representations of the stochastic thermodynamics encoded in the FPE. Specifically, we show in the following how to numerically compute moment generating functions (MGFs) and large-deviation functions (LDFs) of functionals defined along the stochastic trajectories. The analogous procedure for the characteristic function (CHF) could be of interest in cases when the probability density and/or the MGF do not exist. A physical example of some importance in stochastic thermodynamics is the fluctuating efficiency [27–29]. Inspired by such applications, we consider here and in the following section the functionals of work w and heat q along the trajectory x(t), namely

\[ w(\tau) \equiv \int_0^\tau dt \dot{U}(x(t))|_{x=x(t)} = \int_0^\tau dt \dot{k}(t)x^4(t)/4 \]  
\[ q(\tau) \equiv [U(x(\tau), \tau) - U(x(0), 0)] - w(\tau). \]

More precisely, they correspond to the cumulative external work performed on the active particle by the device varying the confinement strength, and the cumulative heat transferred to it by the reservoir, respectively. Here and below, both are understood to be defined (and integrated) along the limit-cycle trajectory \[ x(t) \] for one limit cycle, as computed from BD simulations (symbols) and the 10-100 times faster MNM (lines): a) moments \( \langle x^2 \rangle \), \( \langle x \cos \theta \rangle \) and \( \langle x^4 \rangle \); b) marginal probability density for the particle position at five time-instants during the cycle [note that \( \xi(x, 0) = \xi(x, 1) \)].

Again, as described in Sec. III we approximate the actual driving by one that is piece-wise constant. Such a protocol is highly suitable for the calculation of work and heat distributions. According to Eq. (14), work is only done on the system at instants \( t = i \Delta_t \), \( i = 2, \ldots, (N_t + 1) \), when the potential abruptly changes. Complementary, heat only flows into the system during time intervals between them. The joint probability distribution for the work and heat absorbed during a time interval \( ((i - 1)\Delta_t, i\Delta_t] \) by the particle starting at position \( x \) at \( t_i = (i - 1)\Delta_t \) and reaching position \( y \) at time \( t_f = i\Delta_t \) is thus given by the weighted product of two δ-functions:

\[ p_i(w, q; x, y) = p(y, t_f; x, t_i)\delta\{w-[U(y, t_f)-U(y, t_i)]\} \times \delta\{q-[U(y, t_i)-U(x, t_i)]\}. \]  

The required probabilities \( p(y, t_f; x, t_i) \) to find the particle starting in \( x \) at time \( t_i \) and finishing in \( y \) at time \( t_f \) are determined by matrix elements of the propagator \( U(t_f, t_i) = U_i \). The probability density \( p_i(w, q; x, y) \) of the full process during the time interval \([0, t]\) can therefore again be constructed from corresponding probabilities for the individual short-time intervals. Such a cal-
calculation, however, involves a large number of convolutions over work and heat transferred during the time increments, which is not easily implemented in practice. But one can get rid of the convolutions using Laplace (or Fourier) transformations and calculate the MGF (or CHF) for work and heat, directly.

In order to do so, it is favorable to construct the so-called tilted propagators \( \hat{U}_t(s_w, s_q) \), where \( s_w \) and \( s_q \) denote the Laplace (or Fourier) variables corresponding to \( w \) and \( q \). The matrix elements of \( \hat{U}_t \) are obtained by multiplying the \((N_0 + 1)^2\) matrix elements of \( U_t \) corresponding to \( p(y, t_f; x, t_i) \) by the Laplace (Fourier) transform of \( \delta \{ w - [U(y, t_f) - U(y, t_i)] \} \delta \{ q - [U(y, t_f) - U(x, t_i)] \} \), which is just a product of two exponentials. In terms of the tilted matrices, the MGF for the whole process is given by

\[
\chi(s_w, s_q) = \mathbf{p}_w^\top \cdot \hat{U}(s_w, s_q) \cdot \mathbf{p}_0 \quad \text{with} \quad \hat{U}(s_w, s_q) \equiv \lim_{\Delta t \to 0} \prod_{i=1}^{N_t} \hat{U}_i(s_w, s_q). \tag{18}
\]

Here \( \mathbf{p}_0 \) is the column vector describing the state of the system at the initial time 0, and \( \mathbf{p}_w^\top \) is a row vector of ones that ensures summation over all final states of the system. In a similar manner it is possible to calculate CHFs and MGFs for other quantities of interest, such as the entropy production or probability current \( \hat{J}_w(t) \), etc.

Using this method, we calculated the MGFs \( \chi_w = \chi(s_w, 0) \) and \( \chi_q = \chi(0, s_q) \) for the work \( \hat{J}_w \) and heat \( \hat{J}_q \) transferred to the active particle during one (limit) cycle, using the discretization and driving protocol described in Sec. \( \text{III} \). The resulting moment generating functions are shown in Fig. \( 5 \). To check the results, we computed the first 11 raw moments using the formula \( \langle y^n \rangle = (-1)^n d^n \hat{g}(s_q) / d s_q^n \) for \( y = w, q \). They are depicted in Fig. \( 5 \) (a) together with the corresponding results obtained from the BD simulations (b). In order to assess the error of the latter, we simulated each moment 10 times using \( 10^6 \) trajectories (yielding 10 symbols for each \( n \) in the figure). For the exchanged work, all * and the corresponding \( \Box \) from the MNM perfectly overlap, for all values of \( n \) (Fig. \( 5 \), left). For the heat, such perfect agreement is limited to \( n = 0 \ldots 4 \) (Fig. \( 5 \), right).

For \( n \geq 5 \), the simulation results (b) cease to overlap, indicating that the heat \( q \) fluctuates more strongly than the work \( w \). Moreover, for \( n > 8 \), the MNM meets the limit of double-precision arithmetics, which causes discrepancies between the MNM results and the BD averages. In contrast to \( \chi_w \), the MGF \( \chi_q \) for heat changes so slowly around \( s_q = 0 \) that 16 significant digits provide insufficient precision for the higher derivatives involved in the calculation of \( \langle q^n \rangle \) for \( n = 9, 10 \).

V. LARGE-DEVIATION FUNCTIONS

The tilted matrices \( \hat{U}_t(s_w, s_q) \) in the Laplace variables \( s_w \) and \( s_q \) can also be used to calculate the large-deviation functions (LDFs) for work and heat. Large-deviation theory \( \text{30} \) assumes that the distribution \( \rho(w, q) \) for the cumulative work and heat supplied to the system during \( N \gg 1 \) cycles can be written in the form \( \rho(w, q) \approx \exp[NJ(w/N, q/N)] \), where the LDF \( J(w, q) = \min_{s_w, s_q} \log \chi(s_w, s_q) + ws_w + qs_q \) follows from the MGF \( \chi(s_w, s_q) \) via a Legendre–Fenchel transformation. The MGF for \( N \) cycles reads \( \chi = \mathbf{p}_w^\top \hat{U}^N \mathbf{p}_0 \). Assuming the eigenvalues of the tilted propagator matrix \( \hat{U}(s_w, s_q) \) to be non-degenerate (well-aged), this implies for \( N \gg 1 \) that \( \log \chi \approx \log \lambda \), where \( \lambda(s_w, s_q) \) is the largest eigenvalue of \( \hat{U}(s_w, s_q) \). To sum up, the LDF for work and heat transferred to the system after many cycles reads

\[
J(w, q) = \min_{s_w, s_q} \log \lambda(s_w, s_q) + ws_w + qs_q. \tag{19}
\]

Via the largest eigenvalue of the tilted matrix \( \hat{U}(s_w, s_q) \), the MNM thus allows for an efficient computation of the LDFs of work and heat. In Fig. \( 6 \) we consider both quantities individually, i.e., we study \( J_w(w) = \min_{s_w} \log \lambda(s_w, 0) + ws_w \) and \( J_q(q) = \min_{s_q} \log \lambda(0, s_q) + qs_q \), separately. For \( N \gg 1 \), the nonextensive boundary term \( U(x, \tau) - U(x, 0) \) in Eqs. \( (15) \)–\( (16) \) can be neglected, so that \( \rho_x(x) \sim \exp[NJ_x(x/N)] \) for \( x = q, -w \), and \( J_q(q) = J_w(-w) \), as is verified by our MNM results (superimposing lines). How-
ever, the data obtained from $10^6$ BD trajectories (symbols) shows that only the work distribution ($\square$) attains the large deviation limit quickly, while the heat distribution ($\bigcirc$) has not converged, even for $N = 100$ cycles.

VI. CONCLUSION AND OUTLOOK

Our numerical scheme shares basic notions with so-called Markov-state models of molecular kinetics, which have been employed for interpreting data from single-molecule experiments and molecular-dynamics simulations [31]. Both methods exploit the mapping of stochastic processes occurring in continuous space and time to discrete state-space Markov processes. While the kinetic Markov-state models are often based on special protocols, such as time-periodic driving [32], our formulation can in principle handle arbitrary time-dependent protocols. It can be further modified, in various ways. For example, one can use a more complicated discrete lattice with position-dependent mesh constants $\Delta_x$ and $\Delta_y$. The method also allows for a straightforward implementation of hard walls and barriers via suitable boundary conditions. For an absorbing boundary and a time-independent potential we refer to a recent study of the dynamics of a particle in an unstable potential [10].

The method is also readily generalized to higher-dimensional problems. The main technical limitation is the available RAM, which determines the largest matrix that can swiftly be handled by the computer. The rate matrix $R$ in Eq. (9) has at most $\prod_{i=1}^{d}(N_i + 1)(1 + 2d)$ nonzero elements, where $d$ denotes the dimensionality of the problem and $N_i + 1$ denotes the number of discrete points considered for the $i$th dimension. This is because each site in Fig. 1 is connected to at most $2d$ neighbors and each of the $\prod_{i=1}^{d}(N_i + 1)$ rows of $R$ thus contains $2d$ rates for transitions into the given site and 1 outward rate. On the other hand, the propagators $U(t, t_0)$ already contain $\prod_{i=1}^{d}(N_i + 1)^2$ nonzero matrix elements. The largest number of nonzero elements which can be handled by our computer (8 GB RAM) is approximately $10^6$. In practice, problems that can be solved solely using the rate matrix $R$, such as the computation of a (non-equilibrium) stationary solution of Eq. (9), can usually be attacked with acceptable precision in higher dimensions, whereas fully time-dependent problems require additional resources.

ACKNOWLEDGMENTS

We thank M. Žonda for valuable comments on a preliminary version of the manuscript. VH gratefully acknowledges support by the Humboldt foundation and by the Czech Science Foundation (project No. 17-06716S). S.S. acknowledges funding by International Max Planck Research Schools (IMPRS).

[1] K. Sekimoto, Stochastic Energetics, Lecture Notes in Physics, Vol. 799 (Springer, 2010).
[2] U. Seifert, Rep. Prog. Phys. 75, 126001 (2012).
[3] T. Speck, EPL (Europhysics Letters) 114, 30006 (2016).
[4] H. Risken, The Fokker-Planck Eq. Methods of Sol. and Appl. (Springer, Berlin, Heidelberg, 1996).
[5] N. V. Kampen, Physics Reports 124, 69 (1985).
[6] R. Friedrich, J. Peinke, M. Sahimi, and M. R. R. Tabar, Physics Reports 506, 87 (2011).
[7] A. Traulsen, J. C. Claussen, and C. Hauert, Phys. Rev. E 85, 041901 (2012).
[8] P. Slanina, Essentials of econophysics modelling (OUP Oxford, 2013).
[9] W. Paul and J. Baschnagel, Stochastic Processes: From Physics to Finance (Springer Berlin Heidelberg, 2010).
[10] A. A. Drgulescu and V. M. Yakovenko, Quantitative Finance 2, 443 (2002).
https://doi.org/10.1080/14697688.2002.0000011
[11] S. Narayanan and P. Kumar, in IUTAM Symposium on Nonlinear Stochastic Dynamics and Control, edited by W. Q. Zhu, Y. K. Lin, and G. Q. Cai (Springer Netherlands, Dordrecht, 2011) pp. 77–86.
[12] B. Sepehrian and M. K. Radpoor, Applied Mathematics and Computation 262, 187 (2015).
[13] L. Pichler, A. Masud, and L. A. Bergman, Computational Methods in Stochastic Dynamics: Volume 2, edited by M. Papadrakakis, G. Stefanou, and V. Pa-
padopoulos (Springer Netherlands, Dordrecht, 2013) pp. 69–85.

[14] V. Holubec, *Non-equilibrium Energy Transformation Processes: Theoretical Description at the Level of Molecular Structures* (Springer, 2014).

[15] S. Das, G. Gompper, and R. G. Winkler, *New Journal of Physics* **20**, 015001 (2018).

[16] L. Ornigotti, A. Ryabov, V. Holubec, and R. Filip, *Phys. Rev. E* **97**, 032127 (2018).

[17] A. Ryabov, V. Holubec, M. H. Yaghoubi, M. Varga, M. E. Foulaadvand, and P. Chvosta, *J. Stat. Mech: Theory Exp.* **2016**, 093202 (2016).

[18] V. Holubec, A. Ryabov, M. H. Yaghoubi, M. Varga, A. Khodaei, M. E. Foulaadvand, and P. Chvosta, *Entropy* **19**, 119 (2017).

[19] M. F. Weber and E. Frey, *Reports on Progress in Physics* **80**, 046601 (2017).

[20] C. Maes and K. Netočný, *Scholarpedia* **8**, 9664 (2013), revision #134780.

[21] P. Romanczuk, M. Bär, W. Ebeling, B. Lindner, and L. Schimansky-Geier, *Eur. Phys. J. Special Topics* **202**, 1 (2012).

[22] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe, *Rev. Mod. Phys.* **88**, 045006 (2016).

[23] G. Gompper, C. Bechinger, S. Herminghaus, R. Isele-Holder, U. B. Kaupp, H. Löwen, H. Stark, and R. G. Winkler, *Europ. Phys. J. Spec. Top.* **225**, 2061 (2016).

[24] V. Blickle and C. Bechinger, *Nature Phys.* **8**, 143 (2012).

[25] I. A. Martínez, É. Roldán, L. Dinis, D. Petrov, J. M. R. Parrondo, and R. A. Rica, *Nature Phys.* **12**, 67 (2016).

[26] S. Krishnamurthy, S. Ghosh, D. Chatterji, R. Ganapathy, and A. K. Sood, *Nat Phys* **12** (2016).

[27] G. Verley, M. Esposito, T. Willaert, and C. Van den Broeck, *Nature Communications* **5** (2014).

[28] M. Polettini, G. Verley, and M. Esposito, *Phys. Rev. Lett.* **114**, 050601 (2015).

[29] K. Proesmans, B. Cleuren, and C. V. den Broeck, *EPL (Europhysics Letters)* **109**, 20004 (2015).

[30] H. Touchette, *Physics Reports* **478**, 1 (2009).

[31] J.-H. Prinz, H. Wu, M. Sarich, B. Keller, M. Senne, M. Held, J. D. Chodera, C. Schütte, and F. Noé, *The Journal of Chemical Physics* **134**, 174105 (2011).

[32] H. Wang and C. Schütte, *J. Chem. Theor. and Comp.* **11**, 1819 (2015).