Patchwork sampling of stochastic differential equations

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We propose a method to sample stationary properties of solutions of stochastic differential equations, which is accurate and efficient if there are rarely visited regions or rare transitions between distinct regions of the state space. The method is based on a complete, nonoverlapping partition of the state space into patches on which the stochastic process is ergodic. On each of these patches we run simulations of the process strictly truncated to the corresponding patch, which allows effective simulations also in rarely visited regions. The correct weight for each patch is obtained by counting the attempted transitions between all different patches. The results are patchworked to cover the whole state space. We extend the concept of truncated Markov chains which is originally formulated for processes which obey detailed balance to processes not fulfilling detailed balance. The method is illustrated by three examples, describing the one-dimensional diffusion of an overdamped particle in a double-well potential, a system of many globally coupled overdamped particles in double-well potentials subject to additive Gaussian white noise, and the overdamped motion of a particle on the circle in a periodic potential subject to a deterministic drift and additive noise. In an appendix we explain how other well-known Markov chain Monte Carlo algorithms can be related to truncated Markov chains.

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I. INTRODUCTION

For ergodic systems it is possible to infer statistical properties by monitoring time series since for large observation times the temporal average of an observable converges to the statistical average. However, in practice the observation time is always finite. Therefore regions of low probability are typically rarely visited within the observation time. Nevertheless they could give substantial contributions to expectation values. This is the problem of rare events or large deviations. A related problem may occur if several regions of large probability are separated by regions of low probability. When starting in one of the regions of large probability the system is typically caught in this region for long times. If the observation time is not long enough other regions are not seen with high probability. We refer to this as the problem of rare transitions.

Time series could be obtained from experiments, observations of natural phenomena, or computer simulations. Computer simulations of stochastic systems are used to access statistical properties and the problem of rare events or rare transitions occurs in many different fields.

Applications in statistical physics include equilibrium phenomena such as phase transitions, especially of first order, or reaction kinetics, as well as nonequilibrium phenomena such as polymer folding and relaxation of spin glasses. Other applications are in queuing theory, for example in communication networks, in supply chain management, and in computation. A detailed review of possible applications is beyond the scope of this paper.

Several simulation techniques have been developed to overcome the problems of rare events or rare transitions and we want to divide them into two categories. As the first category we consider techniques that are designed to estimate the probability of a particular rare event such as first exit events when one is interested in the probability that a certain threshold is passed until a certain time. We consider these as dynamic properties of the system. There is a huge literature on methods of this type and we cannot give a detailed review here. Many of them consider not independent trajectories but generate artificially a family of trajectories with the desired properties suitable to improve the statistics of the rare event. The prevalence of these trajectories should be compensated by properly adjusting their statistical weight. Some examples from this category are [1–5]; cf. also [6,7] for reviews.

As the second category we consider techniques that are designed to estimate only stationary expectation values of observables of the system. Our method is in this category and in the following we will sketch some other methods in this spirit.

A deterministic numerical evaluation of high-dimensional integrals is hardly feasible and Monte Carlo methods are used instead [8]. They appear for example in statistical physics where one is interested in expectation values of observables according to some stationary probability measure on the phase space, the dimension of which is typically a multiple of the number of particles.

When regions of state space that contribute massively to the integral are chosen only with small probability and, on the other hand, regions that contribute only little to the integral are chosen very often, the simulation is inefficient. In importance sampling the sample distribution is modified, such that regions contributing much to the integral are chosen more frequently than regions that contribute almost nothing to the integral. Samples according to the modified distribution might be easier to generate than according to the original distribution. Since one knows how the sample distribution is modified one can reconstruct expectation values according to the original distribution; see Refs. [9,10] for pedagogical introductions. The optimal choice of the sample distribution is discussed, e.g., in [11].

In general, in particular in high dimensions, it is a nontrivial task to efficiently generate a random state according to some given probability distribution. In Markov chain Monte Carlo simulations one uses Markov chains which approach

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asymptotically the desired stationary probability distribution. Examples are Metropolis and Glauber algorithms [12–14].

These methods might suffer the rare event problem as well. Additionally, the Markov chain needs to assume its stationary state reasonably fast. In particular, this is not ensured if there are rare transitions from one frequently visited region into another through a region that is only seldom visited. This happens for instance when sampling with the canonical measure at a first-order phase transition, where a long time is needed to overcome a free energy barrier. Similarly to the aforementioned importance sampling, in Markov chain Monte Carlo simulations there are strategies to overcome this problem by sampling with a modified probability measure that is almost constant over the region of interest. To this purpose the transition probabilities are changed such that the Markov chain has a different stationary probability measure and visits all interesting regions of state space reasonable fast. In multicanonical simulations [15] the transition probabilities are changed after the performance of a simulation and the procedure is iterated. For a statistical physics view see, e.g., [16,17], and for a review from the perspective of telecommunication [18]. In Wang-Landau sampling [19] the transition probabilities are changed continuously and after predefined time periods the strength of the new modifications is reduced in multiple steps. Hence it is a mixture of continuous modifications and an iterative procedure. In [20] the transition probabilities are changed continuously throughout the whole simulation.

A different approach to overcome the problem of rare passages is the replica exchange method. There the state space is enlarged to contain multiple copies of the original system. Then a Markov chain on this enlarged state space which has different transition probabilities on each copy of the original system is used, thus leading to different stationary measures on different copies. Additionally to the dynamics on each copy, the configurations of the copies are exchanged with a probability depending on the configuration of these copies thus enabling rare passages [21].

The methods of Refs. [15,19,20] are based on the modification of Markov chains that are obtained through certain changes in the transition probabilities. Formally, the modified processes can be seen as truncated Markov chains [22].

In this paper we are interested in stochastic differential equations (SDEs) where obviously also rare events or rare transitions may occur but we are not aware of specialized methods investigating stationary properties in this context [23]. We use a decomposition of the state space into nonoverlapping patches to sample the stationary probability density of SDEs. We simulate the processes strictly truncated to each of this patches. Eventually we assemble data from the simulations of all patches and average them with the correct weights obtained from the number of attempted transitions between different patches. With this patchwork we obtain mean values according to the stationary measure of the original process. If the decomposition is chosen in an advantageous way one can overcome the problems caused by rare transitions and efficiently sample the whole state space. We emphasize that our technique is not able to obtain the probability of arbitrary nonstationary rare events such as first exits but it is designed to obtain expectation values according to the stationary measure without the need to wait for the rare events. The mean first passage time, however, can be obtained from the stationary probability density.

The theory of truncated Markov processes is originally formulated for reversible processes [22]. We generalize the procedure to chains that do not satisfy detailed balance. If both forward and time reversed processes can be sampled, patchwork sampling can be performed as well, with a slightly modified version of the truncated process.

The paper is organized as follows. In Sec. II we recall the notion of time reversal for stochastic processes. In Sec. III we introduce our simulation method for reversible Markov chains and apply it to a simple one-dimensional SDE describing the diffusion of an overdamped particle in a double-well potential. As a second example we consider a system of many globally coupled overdamped particles in double-well potentials subject to additive Gaussian white noise which shows a phase transition in the thermodynamic limit [24]. In Sec. IV we generalize the method to systems without detailed balance and apply it to a simple one-dimensional proof of principle system, the overdamped motion of a particles on the circle in a periodic potential subject to deterministic drift and additive noise. In the Appendix we explain the connection of truncated Markov chains with simulation methods that use modified transition probabilities, such as multicanonical or Wang-Landau sampling.

II. TIME REVERSAL

We consider an irreducible, positive recurrent, time homogeneous Markov chain x_t with countable state space X. That means every state $x \in X$ is reached almost surely in finite time. When the initial positions are drawn from the unique invariant measure Π,x_t is a stationary stochastic process. We can consider this stationary process for all $t \in \mathbb{Z}$.

For an arbitrary $\tau \in \mathbb{Z}$ we can define the time reversed process $\tilde{x}_t$ for each realization ω as

$$\tilde{x}_t(\omega) = x_{\tau - t}(\omega). \tag{1}$$

The Markov chain is called reversible if the original process x_t and the time reversed process $\tilde{x}_t$ have the same statistical properties. That is for every $n \in \mathbb{N}$,x_0,x_1, ...,x_n have the same joint probability distribution as x_n,x_{n-1}, ...,x_0. This means that due to homogeneity x_0,x_1, ...,x_n and $\tilde{x}_0$,$\tilde{x}_1$, ...,$\tilde{x}_n$ have the same joint distribution.

The process x_t is reversible if and only if the detailed balance condition

$$P(y|x)\Pi(x) = P(x|y)\Pi(y) \tag{2}$$

is satisfied, where $P(\cdot|\cdot)$ denotes the transition probability

$$P(y|x) = \Pr(x_{t+1} = y | x_t = x) \tag{3}$$

and $\Pi(x)$ is the stationary measure of x_t. If the process x_t is not reversible, the time reversed process $\tilde{x}_t$ is still a well defined irreducible, positive recurrent time homogeneous Markov chain and it has by construction the same unique stationary probability measure Π as the forward process x_t.

III. REVERSIBLE PROCESSES

At the beginning of this section we want to give an intuitive picture, which serves as a guideline in the following constructions. Imagine we want to obtain, by simulations, the expectation value of some quantity, given that the system is in some particular subset of all possible states. If we use a Markov chain to sample the system, it might leave the region of interest. To collect more data we have to wait until the Markov chain returns. In principle we want to leave out all the steps that the Markov chain performs out of the region of interest and continue immediately at the point when the Markov chain returns. The problem is that we do not know at which position it will return, unless we have simulated the whole trajectory. Fortunately we do not need the position of the return point of exactly this trajectory. Since we are interested only in statistical averages it is enough if the return position is chosen with the right probability distribution. As it turns out, for reversible processes the stationary distribution of the return points equals the stationary distribution of the position immediately before the process leaves the region of interest. Hence, each time the Markov chain leaves the region of interest, we put it back to the previous position. In the long time limit we obtain the correct average quantities by this procedure. In the following we want to formalize this procedure and show rigorously its applicability.

We consider an irreducible, stationary, reversible Markov chain $x_t, t \in \mathbb{Z}, x_t \in X$. For simplicity we further assume by now that the state space X is countable. We will comment before subsection A on how the procedure is generalized to continuous systems.

A partition of the state space X is a collection of finitely many, disjoint subsets $(X_1, \ldots, X_N)$ such that $X = \bigcup_{j=1}^{N} X_j$ and all the X_j are measurable with $\Pr(x_t \in X_j) > 0$. A partition is called ergodic if for all j there is a positive probability to reach any point in X_j from any other point in X_j in finite time without leaving X_j in between. That is for any $x_{\text{initial}}, x_{\text{final}} \in X_j$ for all j there exists some $k \in \mathbb{N}$ such that the probability to stay in X_j until $t = k$ and to hit x_{final} at $t = k$ is nonzero,

$$\Pr(x_t \in X_j \text{ for } 0 < t < k, x_k = x_{\text{final}} | x_0 = x_{\text{initial}}) > 0. \quad (4)$$

We construct a new Markov chain, the truncated process $\hat{x}_t$, by modifying the transition probabilities from $x \in X_j$ to $y \notin X_j$, where X_j is from an ergodic partition $(X_1, \ldots, X_N)$ of the state space, as follows:

$$\widehat{P}(y|x) = c\, P(y|x), \quad (5)$$

$$\widehat{P}(x|x) = P(x|x) + (1-c) \sum_{y' \notin X_j} P(y'|x), \quad (6)$$

with $c \in [0,1)$; all other transition probabilities remain unchanged. One easily checks that the modified transition probabilities conserve probability; that is,

$$\sum_{y \in X} \widehat{P}(y|x) = 1 \quad (7)$$

for all $x \in X$. If we find a probability measure $\widehat{\Pi}_j$ of $\hat{x}_t$ that satisfies detailed balance

$$\widehat{P}(y|x)\widehat{\Pi}_j(x) = \widehat{P}(x|y)\widehat{\Pi}_j(y), \quad (8)$$

it must be the unique stationary measure of $\hat{x}_t$. We easily check that

$$\widehat{\Pi}_j(x) = \frac{1}{Z_c}\Pi(x) \times \begin{cases} 1, & \text{for } x \in X_j, \\ c, & \text{for } x \notin X_j, \end{cases} \quad (9)$$

with normalization $Z_c = c\,\Pi(X \setminus X_j) + \Pi(X_j)$ is indeed a solution of Eq. (8) when inserting Eqs. (5) and (6) into Eq. (8) and using Eq. (2). In Kelly [22], chapter 1.6, an analog expression for Markov processes with continuous time is given where the transition rates are modified.

For $c \neq 0$ these truncated processes can be used to construct simulation techniques such as [15,19]. In the Appendix we explicitly demonstrate the connection of these methods with the truncated processes.

For $c = 0$ the process $\hat{x}_t$ is strictly truncated to X_j, i.e., the measure $\widehat{\Pi}(X \setminus X_j)$ is zero, and for $x \in X_j$ we have

$$\widehat{\Pi}_j(x) = \frac{\Pi(x)}{\Pi(X_j)} = \Pr(x | x \in X_j), \quad (10)$$

where $\Pr(\cdot|\cdot)$ denotes the conditional probability of the original process. In practice we generate trajectories of the strictly truncated process $\hat{x}_t$ by running a numerical scheme for the original process x_t with initial value in X_j. Each time t' when the process leaves X_j, that is, $x_{t'} \notin X_j$, we artificially set $\hat{x}_{t'} = x_{t'-1}$ and continue with a new realization of x which agrees with $\hat{x}$ at time t'. Constructed in this way $\hat{x}_t$ is a Markov chain living on X_j with transition probabilities $\widehat{P}(\cdot|\cdot)$ defined above. The procedure is illustrated in Fig. 1.

In this paper we devise a simulation method exploiting the case $c = 0$. We sample the strictly truncated process for each X_j of an ergodic partition and multiply the obtained expectation values with the corresponding weights $\Pi(X_j)$. Summing these weighted expectation values we obtain expectation values according to the stationary probability distribution of

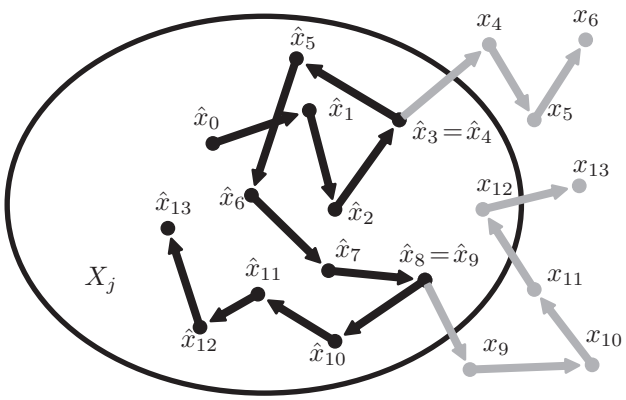

FIG. 1. Construction of the strictly truncated process $\hat{x}_t$. Inside X_j the process follows realizations of x_t. Each time x_t leaves X_j the truncated process is set back to its previous position and follows a new realization of x_t. Note that the two gray paths leaving X_j are different realizations of x_t.

the original process, i.e.,

$$\sum_{j=1}^{N} \langle \mathcal{O} \rangle_{X_j} \Pi(X_j) = \langle \mathcal{O} \rangle_X, \tag{11}$$

where $\mathcal{O}(x)$ denotes an observable, $\langle \cdot \rangle_{X_j}$ is the expectation value according to the stationary measure $\widehat{\Pi}_j(x)$ of the process strictly truncated to X_j, and $\langle \cdot \rangle_X$ is the expectation value according to the stationary measure $\Pi(x)$ of the original process. The advantage of this method is that we can easily obtain data also from regions of state space that are rarely visited by the original process.

To reconstruct the expectation values of the original process according to Eq. (11) we need to know the weights $\Pi(X_j)$. They can be estimated directly from the simulation of the strictly truncated processes exploiting detailed balance without the need to simulate the original process. From Eq. (2) it follows that

$$\sum_{y \in X_k} \sum_{x \in X_j} P(y|x)\Pi(x) = \sum_{x \in X_j} \sum_{y \in X_k} P(x|y)\Pi(y). \tag{12}$$

That is, the probability that $x_t \in X_j$ and $x_{t+1} \in X_k$ equals the probability that $x_t \in X_k$ and $x_{t+1} \in X_j$. Introducing the transition indicator

$$\mathbb{1}_{kj}(x_{t+1}, x_t) = \begin{cases} 1, \text{ if } x_t \in X_j \text{ and } x_{t+1} \in X_k, \\ 0, \text{ else,} \end{cases} \tag{13}$$

we can rewrite Eq. (12) with the help of Eq. (10) in terms of the expectation of the transition indicators as

$$\langle \mathbb{1}_{kj} \rangle_{X_j} \Pi(X_j) = \langle \mathbb{1}_{jk} \rangle_{X_k} \Pi(X_k). \tag{14}$$

During the simulation of the strictly truncated process we count how often the original process tries a forbidden transition from X_j into X_k and denote this number as $n_{kj}(t) = \sum_{t'=0}^{t-1} \mathbb{1}_{kj}(x_{t'+1}, x_{t'})$. The quantity $n_{kj}(t)/t$ is a time average of $\mathbb{1}_{kj}$. Hence due to ergodicity we have

$$\langle \mathbb{1}_{kj} \rangle_{X_j} = \lim_{t \to \infty} \frac{n_{kj}(t)}{t}. \tag{15}$$

Therefore, according to Eq. (14), for large t we can estimate

$$\Pi(X_j)/\Pi(X_k) \approx n_{jk}(t)/n_{kj}(t). \tag{16}$$

Together with the normalization condition

$$\sum_{j=1}^{N} \Pi(X_j) = 1 \tag{17}$$

we find estimates for the weights $\Pi(X_j)$.

We have formulated the simulation method for Markov chains with countable state space X and discrete time. However our main interest is to generate solution trajectories of SDEs where both state space and time are continuous.

We nevertheless apply the method, as established methods discretize the time anyway, e.g., the Euler-Maruyama scheme [25]. A rigorous generalization to systems with continuous time could be a topic of further research. We did not try this here since all our simulations rely on discrete time.

For our argument we used the Markov property, the existence of a unique stationary measure, and further that this measure is approached asymptotically for $t \to \infty$, which is ensured when the state space is countable. However the same properties follow for a continuous state space, when x_t is a recurrent aperiodic Harris chain; see, e.g., [26,27]. The time discretization scheme for SDEs used in this paper is a Harris chain [28] and hence the method can be applied.

We further remark that all simulations performed on a real computer use in fact a discretization in space due to the finite resolution of floating point numbers. This discretization in space might cause additional problems in particular with respect to the Markov property. However, these problems are not related to the method of patchwork sampling but appear for any simulation when implemented on digital computers.

A. Introductory example

Consider the Langevin equation

$$\dot{x} = -\frac{\partial}{\partial x} U(x) + \xi(t), \tag{18}$$

with

$$U(x) = -\frac{a}{2}x^2 + \frac{1}{4}x^4, \tag{19}$$

where $x \in \mathbb{R}$ and $\xi(t)$ is Gaussian white noise satisfying

$$\langle \xi(t)\xi(s) \rangle = \sigma^2 \delta(t-s), \tag{20}$$

where $\langle \cdot \rangle$ denotes the average with respect to all realizations of ξ.

The stationary probability density of the process x_t described by Eq. (18) is

$$p_s(x) = \frac{1}{Z} \exp\left[-\frac{2}{\sigma^2} U(x)\right], \tag{21}$$

where Z is the normalization.

We want to sample the trajectories of (18) with the Euler-Maruyama scheme

$$x(t+\Delta t) = x(t) + [ax(t) - x^3(t)]\Delta t + \sigma\sqrt{\Delta t}\,\eta(t), \tag{22}$$

where $\eta(t)$ are independent Gaussian random variables with zero mean and variance 1. Equation (22) is an approximation of Eq. (18) which becomes exact for $\Delta t \to 0$. The scheme is equivalent to the Milstein scheme since there is only additive noise. The strong and the weak order of the scheme is 1; cf. [25].

For $a > 0$ the probability density (21) is bimodal. For large a or small σ, sampling $p_s(x)$ with the scheme (22) might not lead to satisfying results because in that case the mean first passage time to go from the potential minimum at $x = \sqrt{a}$ over the potential barrier at $x = 0$ is exponentially large. According to Kramers [29] we have

$$\begin{aligned} \tau_{\text{mfp}} &\approx \frac{\pi\sigma^2}{\sqrt{-U''(\sqrt{a})U''(0)}} \exp(2/\sigma^2 \Delta U) \\ &= \frac{\pi\sigma^2}{\sqrt{2}a} \exp[a^2/(2\sigma^2)], \end{aligned} \tag{23}$$

with $\Delta U = U(0) - U(\sqrt{a})$. This time is exponentially large in $(a/\sigma)^2$. Hence it can easily be larger than any in practice accessible simulation time such that starting in the vicinity of $\sqrt{a}$ we do not see the peak at $-\sqrt{a}$ in the simulation when

naively applying Eq. (22). In this case the standard approach is not at all applicable to sample the stationary distribution.

In this example the state space is $X = \mathbb{R}$. To demonstrate the advantage of the method we use the partition $(X_1, \ldots, X_{32})$ with $X_1 = (-\infty, -3.5), X_{32} = [3.5, \infty)$ and the other X_j are intervals of equal length such that $[-3.5, 3.5) = \bigcup_{i=2}^{31} X_i$. This partition is ergodic since each point of any interval can be reached without leaving the interval before. We simulate the processes $\hat{x}_t$ truncated to X_j and find from simulation histograms estimates of the truncated density; cf. Eq. (10). Using Eq. (16) we determine estimates for the probability ratios of adjacent intervals $R_{i,i+1} = \Pi(X_{i+1})/\Pi(X_i), i = 1, \ldots, N-1$. From these ratios we can deduce the probability ratios of two arbitrary intervals, e.g.,

$$R_{1,k} = \prod_{l=2}^{k} R_{l-1,l} = \Pi(X_k)/\Pi(X_1) \quad \text{for } k > 1. \tag{24}$$

Using the normalization condition (17) we obtain estimates for all the $\Pi(X_j)$ according to

$$\Pi(X_i) = R_{1,i} \Big/ \left(1 + \sum_{k=2}^{N} R_{1,k}\right). \tag{25}$$

Hence we can reconstruct $\Pi(x)$ from the truncated probability densities (10) according to

$$\Pi(x) = \sum_{j=1}^{N} \widehat{\Pi}_j(x) \Pi(X_j). \tag{26}$$

In Fig. 2 we see the stationary probability density. The density is approximated by a histogram of the coordinate x, where we considered the indicator function of each histogram bin as an observable, such that the technique of patchwork sampling can be applied. Results of the simulation are compared with a conventional simulation, and with the analytical result. The total number of time steps and hence the computational effort used in the decomposition method and in the conventional simulation are equal. The decomposition method reproduces the analytically known stationary probability density over several orders of magnitude. The conventional simulation, starting at $x_0 = 1$, samples only the positive peak. According to Eq. (23) the mean first passage time over the potential barrier is $\tau_{\text{mfp}} \approx 5.9 \times 10^{10}$; hence it is four to five orders of magnitude larger than the simulation time used. Thus the conventional method cannot reproduce the full stationary probability density.

B. High-dimensional example

We investigate an array of L stochastic, harmonically coupled nonlinear constituents in global coupling under the influence of additive noise, given by the system of Langevin equations

$$\dot{x}_i = a x_i - x_i^3 - \frac{D}{L-1} \sum_{j=1}^{L} (x_i - x_j) + \xi_i \tag{27}$$

for $i = 1, \ldots, L$. Here we consider a as the control parameter. The strength of spatial interaction is controlled by D. The ξ_i

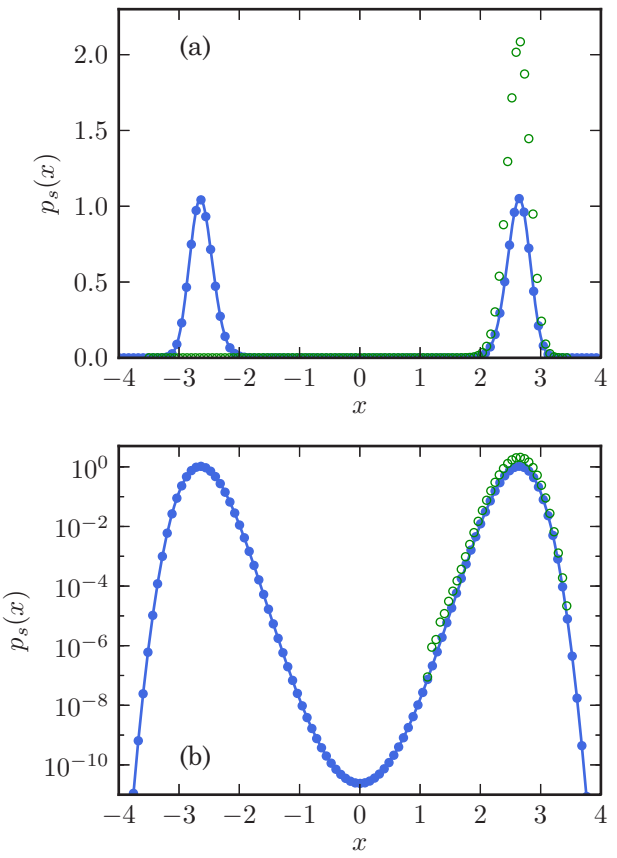

FIG. 2. Stationary probability density $p_s(x)$ of the process (18) for parameters $a = 7, \sigma = 1$. Analytical solution given by Eq. (21) (blue line), conventional simulation (green circles) starting at $x_0 = 1$ with 3×10^9 time steps after a equilibration period of 6×10^8, simulation by decomposition of state space (filled blue circles) with 10^8 time steps for each interval after an equilibration period of 2×10^7 steps. Step size in all simulations was $\Delta t = 10^{-4}$, bin size = 0.007. Note that in the conventional simulation the left peak is completely missed. The same data are displayed on a linear (a) and a logarithmic (b) scale. The logarithmic plot demonstrates perfect agreement of our data with analytical results over 10 orders of magnitude.

are additive zero mean spatially uncorrelated Gaussian white noise processes with autocorrelation function

$$\langle \xi_i(t) \xi_j(t') \rangle = \sigma^2 \delta_{ij} \delta(t - t'); \tag{28}$$

σ is the noise strength. The corresponding Fokker-Planck equation is

$$\partial_t p(\mathbf{x},t) = \sum_{i=1}^{L} -\partial_{x_i} \left\{ \left[(a - D) x_i - x_i^3 + \frac{D}{L-1} \sum_{j=1}^{L} x_j - \frac{\sigma^2}{2} \partial_{x_i} \right] p(\mathbf{x},t) \right\}, \tag{29}$$

where $\mathbf{x}$ is the vector consisting of the coordinates x_i.

This system was studied intensively, in particular in the limit $L \to \infty$ [24,30–34]. In this limit the center of mass R_L

becomes deterministic and is called the mean field:

$$m = \lim_{L\to\infty} R_L = \lim_{L\to\infty} \frac{1}{L}\sum_{i=1}^{L} x_i. \tag{30}$$

In the stable stationary state, m is either zero or assumes one of the values $m_+ = -m_-$. The transition from one to two stable solutions occurs at a critical point $a = a_c$ [24]. The critical point can be calculated numerically by evaluating the phase transition condition [24].

For finite L the full stationary solution of (29) is

$$p_s(\mathbf{x}) = \frac{1}{Z}\exp\left\{-\frac{2}{\sigma^2}\sum_{i=1}^{L}\left[-\frac{a-D}{2}x_i^2 + \frac{1}{4}x_i^4 - \frac{D}{L-1}\sum_{j\neq i} x_j\right]\right\} \tag{31}$$

with normalization Z.

The stationary distribution of the center of mass

$$p_{s,R}(R) = \int_{\mathbb{R}^L} d\, p_s(\mathbf{x})\,\delta\left(R - \frac{1}{L}\sum_{i=1}^{L} x_i\right) \tag{32}$$

cannot easily be evaluated either analytically or numerically. Hence it is interesting to access this distribution by simulations. For the parameter regime where the stable solutions of the infinite system satisfy $m = 0$ we expect a single-peak distribution centered around zero for the finite system. When the infinite system has two stable solutions $m = \pm m_+$ we expect a double-peak distribution centered around $\pm m_+$ for the finite system.

To apply the simulation method, we use the following decomposition of the state space $X = \mathbb{R}^L$, where we make use of the high symmetry of the system. A configuration $\mathbf{x}(t)$ is in the set X_k if there are exactly k coordinates with $x_i(t) < 0$. Hence $k \in \{0,\ldots,L\}$. The sets X_k are invariant under permutations of the coordinates because only the number of coordinates that are smaller than zero determines whether a configuration belongs to X_k. We decompose the sets X_k further as $X_k = Y_k \cup Z_k$, where $\mathbf{x} \in X_k$ is in Y_k if $x_1 < 0$ and it is in Z_k if $x_1 \geqslant 0$. Hence

$$X = \bigcup_{k=0}^{L} X_k = \bigcup_{k=0}^{L}(Y_k \cup Z_k) \tag{33}$$

is a disjoint decomposition of the state space. Note that Y_0 and Z_N are empty. Let

$$\begin{aligned}\widehat{\Pi}_k^Y(\mathbf{x}) &= \Pi(\mathbf{x})/\Pi(Y_k) \text{ for } \mathbf{x} \in Y_k,\\ \widehat{\Pi}_k^Z(\mathbf{x}) &= \Pi(\mathbf{x})/\Pi(Z_k) \text{ for } \mathbf{x} \in Z_k\end{aligned} \tag{34}$$

denote the stationary measures of the processes truncated to Y_k and Z_k, respectively.

In order to obtain the weights $\Pi(Y_k)$ and $\Pi(Z_k)$ we count the transition attempts $m_k(t)$ from Z_k to Y_{k+1} and the number of transition attempts $\widetilde{m}_k(t)$ from Y_{k+1} to Z_k. These are the attempts of x_1 to change sign while the number of other coordinates which are smaller than zero remains constant. Due to detailed balance it holds, cf. Eq. (12),

$$\begin{aligned}\sum_{\mathbf{y}\in Y_{k+1}}\sum_{\mathbf{x}\in Z_k} P(\mathbf{y}|\mathbf{x})\Pi(\mathbf{x}) &= \sum_{\mathbf{x}\in Z_k}\sum_{\mathbf{y}\in Y_{k+1}} P(\mathbf{x}|\mathbf{y})\Pi(\mathbf{y})\\ &= \langle m_k(1)\rangle_{Z_k}\Pi(Z_k)\\ &= \langle \widetilde{m}_k(1)\rangle_{Y_{k+1}}\Pi(Y_{k+1}).\end{aligned} \tag{35}$$

Due to ergodicity this is equivalent to, cf. Eq. (16),

$$\frac{\Pi(Z_k)}{\Pi(Y_{k+1})} = \lim_{t\to\infty}\frac{\widetilde{m}_k(t)}{m_k(t)} \tag{36}$$

for the number of transition attempts of the truncated processes. Furthermore we use a symmetry argument to justify that

$$\begin{aligned}\Pi(Y_k) &= \frac{k}{L}\Pi(X_k),\\ \Pi(Z_k) &= \frac{L-k}{L}\Pi(X_k).\end{aligned} \tag{37}$$

Since the Fokker-Planck equation (29) is symmetric with respect to any permutation of the coordinates also the stationary measure Π has this symmetry. Taking any configuration from X_k and permuting the coordinates with a randomly chosen permutation we will end up in Y_k with probability $\frac{k}{L}$ and in Z_k with probability $\frac{L-k}{L}$.

Given the ratios $\widetilde{m}_k(t)/m_k(t)$ Eqs. (36) and (37) form a system of linear equations. With the normalization condition $\sum_{k=0}^{L}[\Pi(Y_k) + \Pi(Z_k)] = 1$ one can, in principle, solve it to obtain $\Pi(Y_k)$ and $\Pi(Z_k)$. However the transitions from Y_{k+1} to Z_k and vice versa are rare; it takes a long time until x_1 changes its sign. The accuracy of the measured estimates of the expectation values in (35) can be improved dramatically truncating the truncated processes another time.

We choose an ordered set of numbers $0 = s_0 < s_1 < \cdots < s_{N-1} < \infty$ and decompose the negative half line as

$$(-\infty, 0) = \bigcup_{l=1}^{N} I_l, \tag{38}$$

where $I_l = [-s_l, -s_{l-1})$ for $l = 1,\ldots,N-1$ and $I_N = (-\infty, -s_{N-1})$. Similarly for the positive half line

$$[0,\infty) = \bigcup_{l=1}^{N} J_l, \tag{39}$$

where $J_l = [s_{l-1}, s_l)$ for $l = 1,\ldots,N-1$ and $J_N = [s_{N-1},\infty)$. We define the sets

$$\begin{aligned}Y_{kl} &= \{\mathbf{x} \in Y_k | x_1 \in I_l\},\\ Z_{kl} &= \{\mathbf{x} \in Z_k | x_1 \in J_l\}\end{aligned} \tag{40}$$

for $k = 0,\ldots,L$ and $l = 1,\ldots,N$ and run a separate simulation for the processes truncated to each of these sets. We consider this as a second truncation as the process truncated to Y_k is truncated another time to Y_{kl} and similarly for Z_k. This second truncation is very similar to the one-dimensional case since only the coordinate x_1 is caught in an interval. We denote the stationary measures of the processes truncated to Y_{kl} or Z_{kl} by $\widehat{\widehat{\Pi}}_{kl}^Y$ and $\widehat{\widehat{\Pi}}_{kl}^Z$, respectively. For the truncation of Y_k Eq. (26)

becomes

$$\widehat{\Pi}_k^Y(\mathbf{x}) = \sum_{l=1}^{N} \widehat{\widehat{\Pi}}_{kl}^Y(\mathbf{x}) \widehat{\Pi}_k^Y(Y_{kl}) \tag{41}$$

and a similar relation is obtained replacing Y by Z[35].

In order to reconstruct the measure $\widehat{\Pi}_k^Y$ we need to estimate the measures of the patches $\widehat{\Pi}_k^Y(Y_{kl})$. Therefore we count the transition attempts $n_{l+1,l}(t)$ from Y_{kl} to Y_{kl+1}. Due to detailed balance we have according to Eq. (16)

$$\frac{\widehat{\Pi}_k^Y(Y_{kl})}{\widehat{\Pi}_k^Y(Y_{kl+1})} = \lim_{t\to\infty} \frac{n_{l,l+1}(t)}{n_{l+1,l}(t)}, \tag{42}$$

normalization implies

$$\sum_{l=1}^{N} \widehat{\Pi}_k^Y(Y_{kl}) = \widehat{\Pi}_k^Y(Y_k) = 1 \tag{43}$$

since the Y_{kl} are disjoint and $\bigcup_{l=1}^{N} Y_{kl} = Y_k$. Similar expressions hold for Z.

We now can obtain the averages of the (possibly rare) events m_k and $\widetilde{m}_k$,

$$\langle m_k(1)\rangle_{Z_k} = \sum_{l=1}^{N} \langle m_k(1)\rangle_{Z_{kl}} \widehat{\Pi}_k^Z(Z_{kl}), \tag{44}$$

$$\langle \widetilde{m}_k(1)\rangle_{Y_k} = \sum_{l=1}^{N} \langle \widetilde{m}_k(1)\rangle_{Y_{kl}} \widehat{\Pi}_k^Y(Y_{kl}), \tag{45}$$

replacing the ensemble averages of the twice truncated process by the time averages as

$$\langle m_k(1)\rangle_{Z_{kl}} = \lim_{t\to\infty} \frac{1}{t} m_k(t)|_{Z_{kl}}, \tag{46}$$

$$\langle \widetilde{m}_k(1)\rangle_{Y_{kl}} = \lim_{t\to\infty} \frac{1}{t} \widetilde{m}_k(t)|_{Y_{kl}}. \tag{47}$$

Transitions in the twice truncated processes are not rare; thus in times t accessible in simulations we can obtain estimates for $\langle m_k(1)\rangle_{Z_k}$ and $\langle \widetilde{m}_k(1)\rangle_{Y_k}$ with reasonable accuracy. With Eqs. (35) and (37) and the normalization $\sum_{k=0}^{L}[\Pi(Y_k) + \Pi(Z_k)] = 1$ we can solve for $\Pi(Y_k)$ and $\Pi(Z_k)$. Hence we obtain also the measures

$$\Pi(Y_{kl}) = \widehat{\Pi}_k^Y(Y_{kl})\Pi(Y_k), \tag{48}$$

$$\Pi(Z_{kl}) = \widehat{\Pi}_k^Z(Z_{kl})\Pi(Z_k). \tag{49}$$

With them we can reconstruct the original measure

$$\Pi(\mathbf{x}) = \sum_{k=0}^{L}\sum_{l=1}^{N} \left[\widehat{\widehat{\Pi}}_{kl}^Y(\mathbf{x})\Pi(Y_{kl}) + \widehat{\widehat{\Pi}}_{kl}^Z(\mathbf{x})\Pi(Z_{kl})\right], \tag{50}$$

and thus obtain the expectation value of any observable

$$\begin{aligned}\langle \mathcal{O}\rangle_X &= \sum_{\mathbf{x}\in X} \mathcal{O}(\mathbf{x})\Pi(\mathbf{x}) \\ &= \sum_{\mathbf{x}\in X} \mathcal{O}(\mathbf{x}) \sum_{k=0}^{L}\sum_{l=1}^{N} \left[\widehat{\widehat{\Pi}}_k^Y(\mathbf{x})\Pi(Y_{kl}) + \widehat{\widehat{\Pi}}_k^Z(\mathbf{x})\Pi(Z_{kl})\right] \\ &= \sum_{k=0}^{L}\sum_{l=1}^{N} \left[\langle \mathcal{O}\rangle_{Y_{kl}}\Pi(Y_{kl}) + \langle \mathcal{O}\rangle_{Z_{kl}}\Pi(Z_{kl})\right]\end{aligned} \tag{51}$$

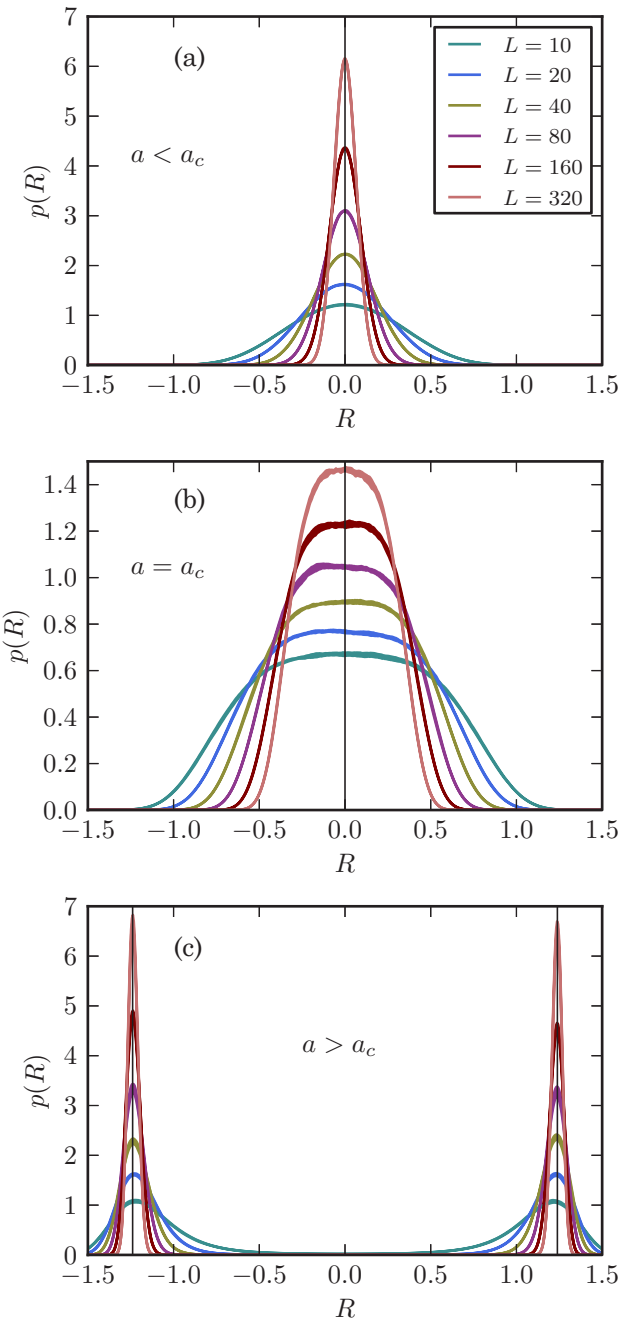

FIG. 3. Distribution of the center of mass coordinate R for system sizes $L = 2^n \times 10$, $n = 0, \ldots, 5$. Sharper distributions correspond to larger system sizes. $a = 0.5$ (a), $a = a_c = 1.078528144127358201 49$ (b), and $a = 2$ (c), $\sigma = 1, D = 1$. Each data set was obtained from five independent realizations of $42 \times L$ simulations with 10^7 recorded time steps ($\Delta t = 10^{-4}$) after an equilibration period of 2×10^6 time steps. The linewidth is twice the standard deviation for each histogram bin (bin size = 0.005). The vertical black lines indicate the stable stationary mean field values of the infinite system.

from the expectation values obtained in the simulations of the twice truncated processes.

We present in Fig. 3 simulation results for the stationary distribution of the center of mass R, i.e., R_L of Eq. (30),

in the subcritical ($a < a_c$), the critical ($a = a_c$), and the supercritical ($a > a_c$) regime. In the subcritical and critical case the distribution has a single peak centered around the stationary mean field of the infinite system ($m = 0$). In the supercritical case there are two stable values for the stationary mean field ($m = \pm m_+$) of the infinite system. For a finite system the center of mass distribution has two peaks centered around these two values. As the system size becomes larger the distributions become narrower in each case. For $a \leqslant a_c$ we characterize fluctuations of R calculating its variance. Since for $a > a_c$ we have a symmetric double-peak distribution for $p_s(R)$, we characterize in this case fluctuations of R as the variance of $|R|$. The shape of the fluctuations of R around its mean field values is Gaussian for $a \neq a_c$ and proportional to $\exp(-\alpha R^4)$ for $a = a_c$ [36]. In the limit $L \to \infty$ fluctuations of the center of mass decay with a power law $L^{-\gamma}$. From the results in [31] describing the scaling of fluctuations of the empirical measure of the x_i one readily derives the exponents $\gamma = 1$ for $a < a_c$ and $\gamma = 1/2$ at $a = a_c$. For $a > a_c$ we expect again $\gamma = 1$ but we are not aware of analytical results in this regime.

Figure 4 shows the fluctuations of R obtained from simulations as a function of the system size L in a log-log plot. The exponent γ was obtained by a linear fit of the data from the four largest system sizes. For $a < a_c$ deviations from the theoretical value for $L \to \infty$ are up to 5%. For $a = a_c$ the deviation is about 6%. For $a > a_c$ the exponent also agrees with the conjectured value $\gamma = 1$ within 5%. Note that the deviations from the theoretical value are essentially not due to inaccuracies in the measurements but are affected by the finite system size since the power law is exact only in the limit $L \to \infty$. Our simulation technique is of similar accuracy in all three cases. In particular the simulation at the critical point is not affected by critical slowing down phenomena.

In the supercritical regime ($a > a_c$) the infinite system faces a breakdown of ergodicity. That is, there are three stationary probability distributions from which two are stable; cf. [24,32,33]. In the long time limit one of these stationary distributions is reached asymptotically. Which of the stationary solutions is obtained depends on initial conditions [37]. The description in, e.g., [32] considers directly the infinite system; that is, it first performs the limit $L \to \infty$ and then investigates stationarity by looking at the limit $t \to \infty$. In our simulations the approach is different as all simulations are done with finite system size. By sampling the stationary distributions we perform, in a sense, the limit $t \to \infty$ first and in a second step we try to notice the limit $L \to \infty$ by investigating larger and larger system sizes. There is no breakdown of ergodicity for any considered finite system. However we see that both peaks of the center of mass distribution become sharper and sharper for larger system sizes. As the probability of the system to be between both peaks decreases we expect that the mean first passage time from one peak to the other diverges which is a harbinger of a breakdown of ergodicity for the infinite system.

We emphasize that the simulation produces only stationary distributions and it cannot estimate the probability of non-stationary rare events. If a realization of a finite but large system is observed for a finite time it is likely to stay close to only one of the peaks throughout the whole observation time. Such a trajectory seems to feel already the ergodicity breaking, since the observation time is not long enough to observe the relaxation to the stationary state, but there is no ergodicity breaking in the finite system in a strict sense. It is important to know the complete stationary distribution when a perturbed system driven by an external time dependent signal is investigated; see, e.g., [38], which allows switching between the two peaks.

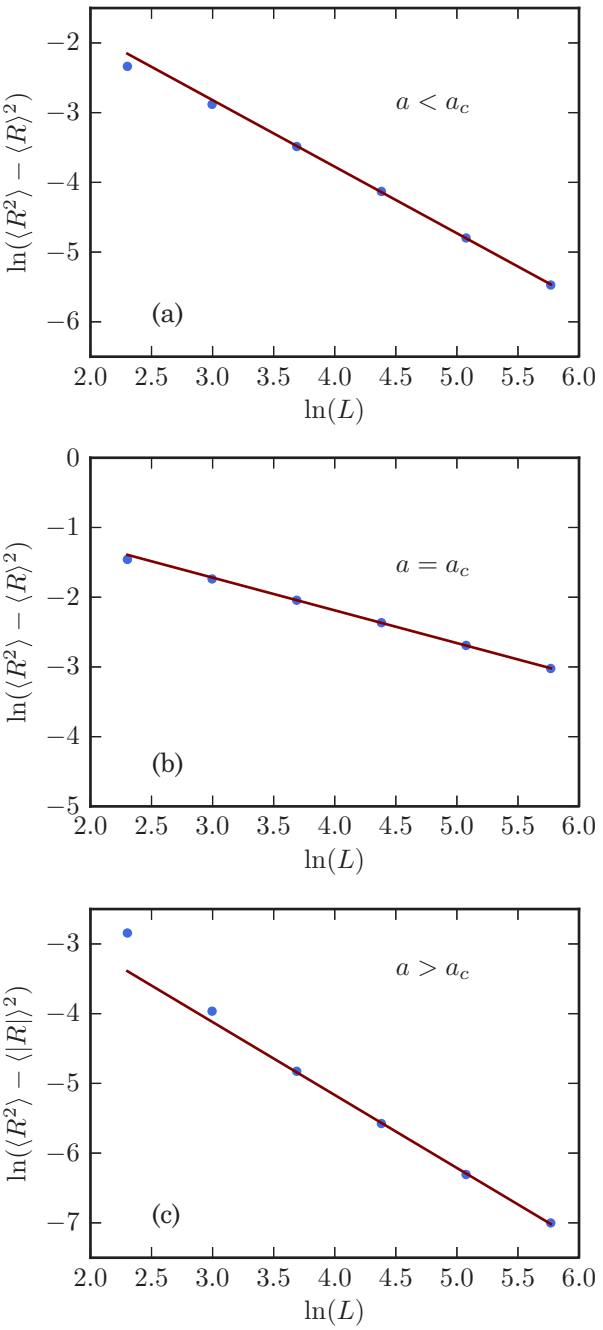

FIG. 4. Fluctuations of the center of mass coordinate R as a function of the system size L averaged over five independent simulations; standard deviations are much smaller than the displayed symbol size. The log-log plots visualize the same data as Fig. 3 and clearly show power laws $L^{-\gamma}$. A linear fit of the four rightmost data points for each simulation gives $\gamma = 0.955(2)$ (a), $\gamma = 0.469(2)$ (b), and $\gamma = 1.046(2)$ (c).

The applicability of the technique hinges on the discovery of an effective partition of the state space. Unfortunately, there is no general recipe that allows one to automatically construct an efficient partition for an arbitrary system, but details of the particular system have to be taken into account. The partition has to be ergodic; i.e., the process truncated to each patch must be ergodic. To make the partition effective there must be a reasonable number of transitions between the patches in order to allow the determination of the corresponding weights with a satisfying accuracy. If the number of transitions is too low, the corresponding patch should be split into two or more. On the other hand, exit attempts should not be the majority of the data. If this is the case either the step size should be reduced or the patch should be unified with another one. In the last example we also used the symmetry of the system. Since all coordinates x_i are equivalent, an exchange between them does not affect macroscopic observables and the division into patches was based on the number of coordinates that lie in certain sets.

IV. NONREVERSIBLE PROCESSES

In this section we generalize the procedure of the previous section to nonreversible Markov processes. Assume we are again in the situation that we want to sample only some part of the configuration space. As before, the Markov process will leave and enter the region of interest and in principle we do not want to waste time simulating the trajectory outside. If the trajectory has left the region of interest, the question remains how to find the position of reentrance without simulating the whole trajectory. Again it is not necessary to obtain the reentrance position of this particular trajectory. It would be enough to choose a position with the correct probability distribution. Unfortunately, the same procedure as for reversible processes does not work in this case, since entrance and exit positions typically have different probability distributions for nonreversible processes. We exploit that time reversal of a trajectory transfers an exit position of the forward process into an entrance position of the backward process. Therefore we use the exit position of the forward process as an initial position of a new realization of the backward process and vice versa. Hence, each time the trajectory leaves the region of interest we continue from the previous position with the reversed process. In the following we will demonstrate that this construction yields the desired statistical properties.

Consider an irreducible stationary Markov process x_t with discrete time $t \in \mathbb{Z}$, defined on a countable state space X with an ergodic partition $(X_1, \ldots, X_N)$ of X. As in Sec. III the procedure can be generalized to Harris chains without any problems, but for simplicity we will only discuss a countable state space here. We denote the time reversed process by $\tilde{x}_t$; cf. Eq. (1).

Consider the forward process x_t that started at $x_0 \in X_j$. The last position of x_t before it leaves X_j the first time will be denoted by y_1^{out}. The position at the first time the process reenters X_j will be denoted by y_1^{in}. The process continues to leave and enter X_j. We denote the corresponding points of the nth exit or entrance by y_n^{out} and y_n^{in}, respectively. Notice that the process leaves or enters the region X_j with probability 1 in finite time. Hence the above construction is reasonable. We can consider the sequences $\{y_n^{\text{out}}\}_{n\in\mathbb{N}}$ and $\{y_n^{\text{in}}\}_{n\in\mathbb{N}}$ as stochastic processes. In fact, they are time homogeneous Markov chains that become stationary in the long time limit. They contain some reduced information of the process x_t similar to Poincaré maps of dynamical systems. The analog construction can be done for the reversed process $\tilde{x}_t$ leading to the reduced processes $\{\tilde{y}_n^{\text{out}}\}_{n\in\mathbb{N}}$ and $\{\tilde{y}_n^{\text{in}}\}_{n\in\mathbb{N}}$.

Since x_t is stationary $\{y_n^{\text{out}}\}_{n\in\mathbb{N}}$ and $\{y_n^{\text{in}}\}_{n\in\mathbb{N}}$ are stationary as well. We denote their stationary distributions by Π^{out} and Π^{in}, respectively. They can be expressed in terms of the original probabilities

$$\Pi^{\text{out}}(y) = \Pr(x_1 = y | x_2 \notin X_j, x_1 \in X_j), \tag{52}$$

$$\Pi^{\text{in}}(y) = \Pr(x_2 = y | x_2 \in X_j, x_1 \notin X_j). \tag{53}$$

By construction we have a relation between the stationary distribution of forward and backward processes, $\forall y \in X_j$:

$$\Pi^{\text{in}}(y) = \widetilde{\Pi}^{\text{out}}(y), \tag{54}$$

$$\Pi^{\text{out}}(y) = \widetilde{\Pi}^{\text{in}}(y). \tag{55}$$

The sequence of random variables $y_1^{\text{out}}, y_1^{\text{in}}, y_2^{\text{out}}, y_2^{\text{in}}, \ldots$ is a time inhomogeneous Markov chain since the transition probabilities from y_n^{out} to y_n^{in} denoted by $F(\cdot|\cdot)$ and from y_n^{in} to y_{n+1}^{out} denoted by $G(\cdot|\cdot)$, which both map $X_j \times X_j \to [0,1]$, differ. We denote the corresponding transition probabilities of the backward process by $\widetilde{F}(\cdot|\cdot)$ and $\widetilde{G}(\cdot|\cdot)$. The form of these transition probabilities is not important for our purposes but it can be given explicitly in terms of conditional probabilities of x_t and $\tilde{x}_t$. For example [39],

$$\begin{aligned} &F\left(y_1^{\text{in}} | y_1^{\text{out}}\right) \\ &= \sum_{k=3}^{\infty} \Pr\left(x_k = y_1^{\text{in}} | x_k \in X_j, \{x_l\}_{l=2}^{k-1} \notin X_j, x_1 = y_1^{\text{out}}\right) \\ &\quad \times \Pr\left(x_k \in X_j, \{x_l\}_{l=3}^{k-1} \notin X_j | x_2 \notin X_j, x_1 = y_1^{\text{out}}\right) \\ &= \sum_{k=3}^{\infty} \Pr\left(x_k = y_1^{\text{in}}, \{x_l\}_{l=3}^{k-1} \notin X_j | x_2 \notin X_j, x_1 = y_1^{\text{out}}\right). \end{aligned} \tag{56}$$

The second line in Eq. (56) is the probability that the process returns to X_j the first time at position y_1^{in} given that the last position in X_j was y_1^{out} and x_t was outside X_j for exactly $k-2$ time steps. The third line gives the probability that x_t remains outside X_j for exactly $k-2$ time steps, given that its last position inside X_j was y_1^{out}. Summing over k we obtain the transition probabilities, since the probability that x_t will never return to X_t is zero. Analogously, the other transition probabilities are

$$\begin{aligned} &G\left(y_2^{\text{out}} | y_1^{\text{in}}\right) \\ &= \sum_{k=3}^{\infty} \Pr\left(x_k \notin X_j, x_{k-1} = y_2^{\text{out}}, \right. \\ &\quad \left. \{x_l\}_{l=3}^{k-2} \in X_j | x_2 = y_1^{\text{in}}, x_1 \notin X_j\right), \end{aligned} \tag{57}$$

$$\widetilde{F}\big(\tilde{y}_1^{\text{in}}|\tilde{y}_1^{\text{out}}\big) = \sum_{k=3}^{\infty} \Pr\big(\tilde{x}_k = \tilde{y}_1^{\text{in}}, \{\tilde{x}_l\}_{l=3}^{k-1} \notin X_j | \tilde{x}_2 \notin X_j, \tilde{x}_1 = \tilde{y}_1^{\text{out}}\big), \quad (58)$$

$$\widetilde{G}\big(\tilde{y}_2^{\text{out}}|\tilde{y}_1^{\text{in}}\big) = \sum_{k=3}^{\infty} \Pr\big(\tilde{x}_k \notin X_j, \tilde{x}_{k-1} = \tilde{y}_2^{\text{out}}, \{\tilde{x}_l\}_{l=3}^{k-2} \in X_j | \tilde{x}_2 = \tilde{y}_1^{\text{in}}, \tilde{x}_1 \notin X_j\big). \quad (59)$$

With $F(\cdot|\cdot)$ and $G(\cdot|\cdot)$ we construct the transition probabilities between two consecutive states of the time homogeneous processes $y_n^{\text{in/out}}$:

$$T^{\text{in}}\big(y_{n+1}^{\text{in}}|y_n^{\text{in}}\big) := \sum_{y\in X_j} F\big(y_{n+1}^{\text{in}}|y\big)G\big(y|y_n^{\text{in}}\big), \quad (60)$$

$$T^{\text{out}}\big(y_{n+1}^{\text{out}}|y_n^{\text{out}}\big) := \sum_{y\in X_j} G\big(y_{n+1}^{\text{out}}|y\big)F\big(y|y_n^{\text{out}}\big). \quad (61)$$

Denote the probability measure of $y_n^{\text{in/out}}$ by $\Pi_n^{\text{in/out}}$ and analogously the probability measures of the backward processes $\tilde{y}_n^{\text{in/out}}$ by $\widetilde{\Pi}_n^{\text{in/out}}$. They satisfy the consistency conditions

$$\Pi_n^{\text{in}}(y) = \sum_{y'\in X_j} F(y|y')\Pi_n^{\text{out}}(y'), \quad (62)$$

$$\Pi_{n+1}^{\text{out}}(y) = \sum_{y'\in X_j} G(y|y')\Pi_n^{\text{in}}(y'), \quad (63)$$

and analogously for the backward process

$$\widetilde{\Pi}_n^{\text{in}}(y) = \sum_{y'\in X_j} \widetilde{F}(y|y')\widetilde{\Pi}_n^{\text{out}}(y'), \quad (64)$$

$$\widetilde{\Pi}_{n+1}^{\text{out}}(y) = \sum_{y'\in X_j} \widetilde{G}(y|y')\widetilde{\Pi}_n^{\text{in}}(y'). \quad (65)$$

We can consider the sets of equations (62) and (63) or (64) and (65) as measure valued dynamical systems. Their fixed points $(\Pi_{\text{fp}}^{\text{in}}, \Pi_{\text{fp}}^{\text{out}})$ and $(\widetilde{\Pi}_{\text{fp}}^{\text{in}}, \widetilde{\Pi}_{\text{fp}}^{\text{out}})$ are just the stationary measures

$$\Pi_{\text{fp}}^{\text{in}} = \Pi^{\text{in}}, \quad (66)$$

$$\Pi_{\text{fp}}^{\text{out}} = \Pi^{\text{out}}, \quad (67)$$

$$\widetilde{\Pi}_{\text{fp}}^{\text{in}} = \widetilde{\Pi}^{\text{in}} = \Pi^{\text{out}}, \quad (68)$$

$$\widetilde{\Pi}_{\text{fp}}^{\text{out}} = \widetilde{\Pi}^{\text{out}} = \Pi^{\text{in}}, \quad (69)$$

where we used the relations (54) and (55) between forward and backward processes.

A new stochastic process z_t^j living on the subset X_j can be constructed in the following way. Given some $x_0 \in X_j$ consider the process x_t started at x_0. Let t_1 be the first time x_t leaves X_j. Set $z_t^j = x_t$ for all $0 \leqslant t < t_1$. Now consider the reversed process $\tilde{x}_t$ started at $z_{t_1-1}^j$ at time t_1 and denote the first time $\tilde{x}_t$ leaves X_j by t_2. Set $z_t^j = \tilde{x}_t$ for all $t_1 \leqslant t < t_2$. Let t_3 be the time the process x_t started at time t_2 at $z_{t_2}^j$ leaves X_j for the first time. Set $z_t^j = x_t$ for all $t_2 \leqslant t < t_3$. Continue in this way switching between realizations of x_t and $\tilde{x}_t$. The construction is illustrated in Fig. 5.

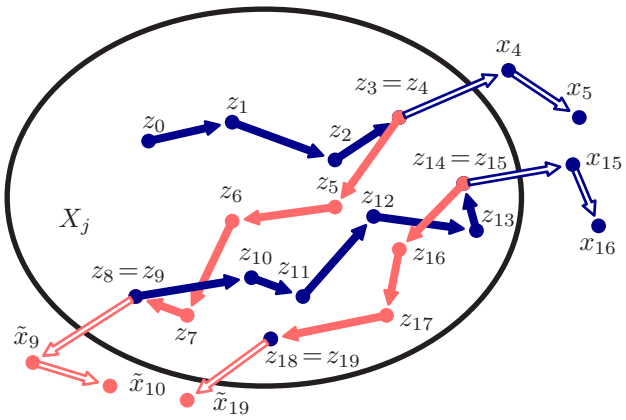

FIG. 5. Construction of the process z_t (filled arrows) from realizations of the forward process x_t (dark blue) and the backward process $\tilde{x}_t$ (dusky pink). Once a realization leaves X_j for the first time it is ignored from then on (illustrated by empty arrows) and the process z_t follows a new realization of the process in the other time direction. Note that the paths leaving X_j are different realizations of x_t or $\tilde{x}_t$.

The process z_t^i is ergodic. It has a unique stationary probability density which is equal to the conditional probability density of the original process x_t given $x_t \in X_i$ as we prove in the following.

In the construction of the process z_t^i we especially consider the times $t_1, t_2, \ldots, t_n$. We denote the positions at these times by $\hat{y}_n := z_{t_n}^i$ and consider even and odd indices separately by introducing $\hat{y}_n^{\text{in}} = \hat{y}_{2n}$ and $\hat{y}_n^{\text{out}} = \hat{y}_{2n-1}$ for $n = 1, 2, \ldots$. These are the last positions of the forward or backward process before it leaves the region X_j. Let $\hat{\Pi}_n^{\text{in/out}}$ be the probability measure of $\hat{y}_n^{\text{in/out}}$. Then the consistency conditions for the processes $\hat{y}_n^{\text{in/out}}$ are

$$\widehat{\Pi}_{n+1}^{\text{out}}(y) = \sum_{y'\in X_j} G(y|y')\widehat{\Pi}_n^{\text{in}}(y'), \quad (70)$$

$$\widehat{\Pi}_n^{\text{in}}(y) = \sum_{y'\in X_j} \widetilde{G}(y|y')\widehat{\Pi}_n^{\text{out}}(y'). \quad (71)$$

Denote the fixed point of these equations by $\widehat{\Pi}_{\text{fp}}^{\text{in/out}}$. Considered as a map of probability measures Eq. (70) is identical to Eq. (63) and Eq. (71) is identical to Eq. (65). Hence we already know a pair of measures that satisfies Eqs. (70) and (71); their fixed point is

$$\big(\widehat{\Pi}_{\text{fp}}^{\text{out}}, \widehat{\Pi}_{\text{fp}}^{\text{in}}\big) = (\Pi^{\text{out}}, \Pi^{\text{in}}). \quad (72)$$

Since $\hat{y}_n^{\text{in/out}}$ have unique stationary measures, this is the unique fixed point. Hence the processes y_n^{in} and $\hat{y}_n^{\text{in}}$ have the same stationary measures as well as the processes y_n^{out} and $\hat{y}_n^{\text{out}}$.

The process z_t is constructed by pieces of realizations of the processes x_t and $\tilde{x}_t$. The initial positions $\hat{y}_n^{\text{in/out}}$ of these pieces are in the long time limit distributed as the initial positions of the original processes x_t or $\tilde{x}_t$. Therefore the distribution of z_t when the time direction is forward will asymptotically

be the same as the distribution of x_t given that $x_t \in X_j$. The distribution of z_t when the time direction is backward is the same as that of $\tilde{x}_t$ given that $\tilde{x}_t \in X_j$. But the stationary distributions of x_t and $\tilde{x}_t$ are the same. Therefore the time direction of z_t is not important and it will be distributed as x_t given $x_t \in X_j$. Note that for a reversible process x_t and $\tilde{x}_t$ are equivalent. Then the process z_t^i is the truncated process; cf. Sec. III.

In order to reconstruct expectation values according to the stationary measure of the original process we need to obtain the weights $\Pi(X_i)$. Similarly to the reversible case we use the number of transition attempts from X_i into X_j. We introduce the transition indicator functions

$$\mathbb{1}_{kj}(x_{t+1},x_t) = \begin{cases} 1, \text{ if } x_t \in X_j \text{ and } x_{t+1} \in X_k, \\ 0, \text{ else,} \end{cases} \tag{73}$$

$$\tilde{\mathbb{1}}_{kj}(\tilde{x}_{t+1},\tilde{x}_t) = \begin{cases} 1, \text{ if } \tilde{x}_t \in X_j \text{ and } \tilde{x}_{t+1} \in X_k, \\ 0, \text{ else,} \end{cases} \tag{74}$$

of the forward and backward process. Since each realization of the backward process can be obtained by time reversal of one realization of the forward process we have for the original forward and backward process

$$\begin{aligned} \langle \mathbb{1}_{kj} \rangle &= \sum_{x\in X_j} \sum_{y\in X_k} P(y|x)\Pi(x) \\ &= \sum_{y\in X_j} \sum_{x\in X_k} \widetilde{P}(y|x)\widetilde{\Pi}(x) = \langle \tilde{\mathbb{1}}_{jk} \rangle. \end{aligned} \tag{75}$$

We can express these expectation values in terms of the truncated process as

$$\langle \mathbb{1}_{kj} \rangle_{X_j} \Pi(X_j) = \langle \mathbb{1}_{kj} \rangle = \langle \tilde{\mathbb{1}}_{jk} \rangle = \langle \tilde{\mathbb{1}}_{jk} \rangle_{X_k} \widetilde{\Pi}(X_k). \tag{76}$$

Counting the number of transition attempts of the forward process n_{kj} and dividing by the number of time steps s in the forward direction is the same as time averaging the transition indicator function $\mathbb{1}_{kj}$; hence

$$\langle \mathbb{1}_{kj} \rangle_{X_j} = \lim_{t\to\infty} \frac{n_{kj}(t)}{s(t)} \tag{77}$$

and analogously for the backward process with the number of time steps in the backward direction $\tilde{s}$:

$$\langle \widetilde{\mathbb{1}}_{jk} \rangle_{X_k} = \lim_{t\to\infty} \frac{\tilde{n}_{jk}(t)}{\tilde{s}(t)}. \tag{78}$$

Since $\lim_{t\to\infty} s(t)/\tilde{s}(t) = 1$ with probability 1, we find with Eq. (76)

$$\Pi(X_j)/\Pi(X_k) \approx \tilde{n}_{jk}(t)/n_{kj}(t), \tag{79}$$

where we used that $\Pi(x) = \widetilde{\Pi}(x)$. Together with the normalization

$$\sum_j \Pi(X_j) = 1 \tag{80}$$

we can estimate the $\Pi(X_j)$ for all j. And expectation values of observables can be obtained from expectation values of the truncated process according to Eq. (11).

In this section we have extended the theory of strictly truncated Markov chains to systems without detailed balance. We remark that it is also possible to construct for nonreversible systems a non-strictly-truncated process that has the stationary measure (9) as in the reversible case. Therefor the construction of the process z_t needs to be slightly modified. Each time the process attempts to leave the set X_j, the step is accepted with probability c. In that case the process continues with a realization of x_t. With probability $1-c$ the escape from X_j is not accepted and the process is set back to the previous position. From then on the process follows a realization of the reversed process $\tilde{x}_t$. Each time when an escape from X_j is not accepted the time direction is reversed. This construction yields the most general version of the truncated process for nonreversible Markov chains. However in this paper we will only use the strictly truncated process.

Example

In the following we will demonstrate the applicability of the method with a simple proof-of-principle example. We aim to construct a one-dimensional, nonreversible system that is as simple as possible but still not totally trivial. Hence we consider an overdamped motion on the circle, described by the angular variable ϕ with additive Gaussian white noise. We will proceed to give the general construction of the time reversed process of such a system, considering the Langevin equation

$$\dot{\phi} = f(\phi) + \xi(t), \tag{81}$$

where $f : [0,2\pi] \to \mathbb{R}$ is a continuous and continuously differentiable function with $f(0) = f(2\pi)$ and $f'(0) = f'(2\pi), \phi \in [0,2\pi]$, and $\xi(t)$ is Gaussian white noise of strength σ. The corresponding Fokker-Planck equation

$$\partial_t p(\phi,t) = -\partial_\phi \left\{ \left[f(\phi) - \tfrac{1}{2}\sigma^2 \partial_\phi \right] p(\phi,t) \right\} \tag{82}$$

with periodic boundary conditions, $p(0,t) = p(2\pi,t)$ and similarly for $\partial_\phi p$, has a unique stationary normalized solution $p_s(\phi)$. We use the stationary solution to define the potential

$$U(\phi) := -\frac{\sigma^2}{2} \ln p_s(\phi) + C, \tag{83}$$

where the constant C can be chosen arbitrarily. With this potential we rewrite the Langevin equation as

$$\dot{\phi} = -\partial_\phi U(\phi) + g(\phi) + \xi(t), \tag{84}$$

where

$$g(\phi) := f(\phi) + \partial_\phi U(\phi). \tag{85}$$

Using this reformulation the stationary Fokker-Planck equation becomes

$$\begin{aligned} 0 = &- \partial_\phi \left\{ \left[-\partial_\phi U(\phi) - \tfrac{1}{2}\sigma^2 \partial_\phi \right] p_s(\phi) \right\} \\ &- \partial_\phi \left[g(\phi) p_s(\phi) \right]. \end{aligned} \tag{86}$$

The term inside the curly brackets is zero by construction of the potential $U(\phi)$. The term on the second line defines the stationary probability current

$$j_{p_s} = g(\phi) p_s(\phi), \tag{87}$$

which must be constant with respect to ϕ in order to satisfy Eq. (86). It is zero if and only if $g(\phi) \equiv 0$, since $p_s(\phi) > 0$ due to the additive noise. If the probability current j_{p_s} is

zero the process is reversible. If it is nonzero the process is not reversible and the time reversed process is obtained by reversing the probability current. Hence the forward process follows Eq. (84) and the time reversed process follows the Langevin equation

$$\dot{\phi} = -\partial_\phi U(\phi) - g(\phi) + \xi(t). \tag{88}$$

In general one would find the potential U and the current term g only after solving the stationary Fokker-Planck equation. This can be done for any function f. As we aim to construct a preferably simple irreversible system we start by choosing the potential

$$U(\phi) = -\frac{A}{3}\cos(3\phi) \tag{89}$$

and the probability current

$$j_{p_s} = \lambda, \tag{90}$$

where $A,\lambda \in \mathbb{R}$ are system parameters. Then the stationary probability distribution

$$p_s(\phi) = \frac{1}{Z}\exp\left[\frac{2}{\sigma^2}\frac{A}{3}\cos(3\phi)\right] \tag{91}$$

with normalization factor Z is independent on the probability current λ. Hence the system describes the overdamped motion in a $-\frac{A}{3}\cos(3\phi)$ potential with an additional constant probability current. The Langevin equation that belongs to the choice (89) and (90) is

$$\dot{\phi} = \lambda Z \exp\left[-\frac{2}{\sigma^2}\frac{A}{3}\cos(3\phi)\right] - A\sin(3\phi) + \xi(t) \tag{92}$$

and the reversed process is obtained replacing λ by $-\lambda$.

This system can easily be simulated using a conventional method, but we use it for a proof of principle of our simulation method for nonreversible systems. The simulation technique developed in this section was applied to simulate the SDE (92). The state space $[0,2\pi]$ was divided into ten intervals of equal size starting with $X_1 = [0,\pi/5)$. We simulated each subset X_i with 10^8 time steps. The simulation results are shown in Fig. 6. There is perfect agreement between the simulation results and the analytic stationary solution (91).

We have demonstrated that for the overdamped motion with force f and additive noise it is always possible to decompose f into a potential part and a part which gives rise to a constant probability current. In higher dimensions there is a similar decomposition of the force into a potential part and a part responsible for a divergence-free probability current density; see for example [40].

V. CONCLUSION

In this paper we have used the concept of truncated reversible Markov processes to develop a simulation technique based on the decomposition of state space. We cut the state space into nonoverlapping patches X_j and run a strictly truncated process on each of them. Expectation values of observables from each of the truncated processes are averaged with the correct weights to obtain expectation values of observables of the original process.

The method collects data from all patches X_j, which is of particular advantage when the original process visits some of these sets only rarely. Furthermore the simulation is parallel; hence all truncated processes can be simulated at the same time. The technique is however restricted to the determination of expectation values according to the stationary measure. It is not suitable to sample the probability of nonstationary rare events, such as first exit events. Contrariwise, it is designed to obtain the stationary properties without the need to wait for the rare events.

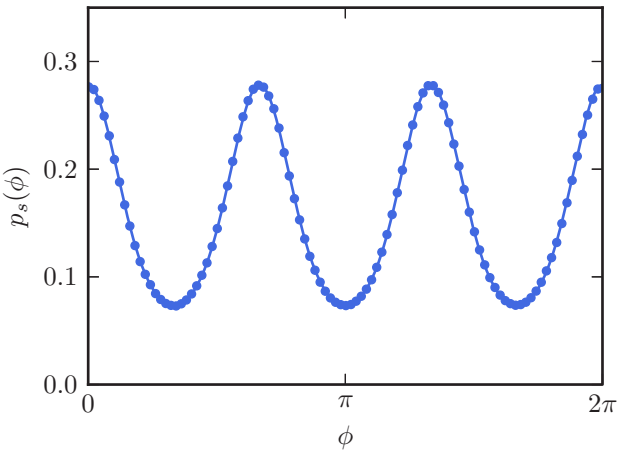

FIG. 6. Stationary probability density $p_s(\phi)$ of the process (92) for parameters $A = 1,\sigma = 1$, and $\lambda = 1$. Analytical solution (blue line) given by Eq. (91) and simulation (filled blue circles) by decomposition of state space into 10 equally sized intervals with 10^8 time steps of size $\Delta t = 10^{-4}$ for each interval. Simulations for other values of λ (2 and 5) give the same results.

We apply the method to stochastic differential equations (SDEs), where we sample the stationary distribution and obtain expectation values of observables. The one-dimensional overdamped motion in a double-well potential with additive Gaussian white noise is used as an introductory example. Already there a conventional simulation fails to sample the double-peak distribution when the potential barrier is too large, whereas our method delivers the correct distribution over ten orders of magnitude.

As a second example a system of L constituents subject to independent additive Gaussian white noise, moving overdamped and globally coupled in the same double-well potential, is simulated. In the limit $L \to \infty$ the center of mass becomes deterministic and has, depending on parameters, one or two stable fixed points. For finite system sizes our simulations produce center of mass distributions that fluctuate around the $L \to \infty$ values. For $a \neq a_c$ these fluctuations are Gaussian whereas at $a = a_c$ they have a distribution $\propto \exp(-\alpha R^4)$. The strength of the fluctuations decays with a power law. The exponents are predicted by theory for $a < a_c$ and $a = a_c$, where they agree with our simulation results. For $a > a_c$ we are not aware of theoretical predictions but we find the same exponent as in the subcritical regime in our simulations. Even at the critical point the simulations are not suffering slowing down effects but produce results almost as accurate as in other parameter regimes.

Furthermore we generalize the concept of truncated Markov chains to ergodic processes that are not reversible. Thereby we are able to transfer the patchwork method to systems without

detailed balance. We apply it to a one-dimensional SDE on the circle that has a constant probability flow in its steady state.

We only use strictly truncated processes for our patchwork simulation technique. However the generalization of the non-strictly-truncated process to systems without detailed balance might be of interest for other simulation methods that implicitly use truncated process and usually require detailed balance.

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APPENDIX: TRUNCATED PROCESSES AND MARKOV CHAIN MONTE CARLO SIMULATIONS

In Sec. III we introduced the truncated process by changing the transition probabilities from one region of state space into another by a factor c. It is possible to repeat this construction with different regions of state space and with different values for c again and again. We give an example construction that eventually leads to a Markov chain as it appears in simulation techniques that sample with a modified probability measure such as [15,19].

We choose a function $f(j)$ for $j \in \{1,\dots,N\}$. In a first step, if $f(1) > f(2)$, we modify the transition probabilities from X_1 into $\bigcup_{l=2}^{N} X_l$ choosing $c = \exp[f(2) - f(1)] < 1$. If $f(1) < f(2)$ we modify the transition probabilities in the other direction, that is from $\bigcup_{l=2}^{N} X_l$ into X_1 choosing $c = \exp[f(1) - f(2)]$. In the next step we manipulate the transition probabilities from $X_1 \cup X_2$ into $\bigcup_{l=3}^{N} X_l$. If $c = \exp[f(3) - f(2)] < 1$ we choose this factor; else we choose the factor $c = \exp[f(2) - f(3)]$ for the transitions in the other direction. We continue to change the transition probabilities between $X_1 \cup X_2 \cup X_3$ and $\bigcup_{l=4}^{N} X_l$ in a similar way. We proceed until we have modified the transition probabilities between $\bigcup_{l=1}^{N-1} X_l$ and X_N. The resulting stationary probability measure satisfies according to Eq. (9)

$$\widehat{\Pi}(X_j) = \frac{1}{Z}\Pi(X_j)\exp[f(j)], \tag{A1}$$

where the normalization Z is such that $\widehat{\Pi}(X) = 1$.

For example, in a Metropolis Monte Carlo simulation in a first step a new state that is chosen at random according to some probability distribution is proposed. In a second step the update is either accepted or rejected with some probability depending on both states. These two steps are repeated.

As the process is constructed here, it might happen that for two configurations x and x' from different sets X_j and $X_{j'}$ there is a nonzero probability of rejection in both directions $x \to x'$ and $x' \to x$. This makes the simulation inefficient. Without changing the stationary measure we can in this case reduce the probability of rejection in both directions by increasing the probabilities of acceptance by the same factor, such that the acceptance probability is 1 in one direction. Doing so, depending on the choice of X_j and f, we end up with a process used, for example, in multicanonical [15] or Wang-Landau [19] simulations. In the multicanonical case the sets X_j consist of all states within some energy interval $[E_j, E_{j+1})$ and the function f is related to the density of states g and the average energy on this interval $f(j) = (E_j + E_{j+1})/2 - \ln g[(E_j + E_{j+1})/2]$, where we assumed for simplicity that the inverse temperature $\beta = 1$. In Wang-Landau sampling the function f is related only to the density of states at the mean energy of the energy interval $f(j) = -\ln g[(E_j + E_{j+1})/2]$. After such a choice of f, in both cases, the process travels to all considered energy intervals with the same probability. Of course, the main ingredient of these methods is to effectively determine the function f from simulations.

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[28] We give the definition of a Harris chain following [27] adopting most of the notation used there. Let (X,S) be a measurable space. We call a Markov chain x_n a Harris chain if there are measurable sets $A,B \in S$, a function $q(x,y) \geqslant \varepsilon > 0$ for $x \in A$ and $y \in B$, and a probability measure ρ on B such that (i) $\Pr_z(\tau_A < \infty) > 0$ for all $z \in X$, where $\tau_A = \inf\{n \geqslant 0 : x_n \in A\}$ and $\Pr_z(\tau_A < \infty) > 0$ denotes the probability that $\tau_A < \infty$ given that $x_0 = z$; (ii) if $x \in A$ and $C \subset B$ then $p(x,C) \geqslant \int_C q(x,y)\rho(d\,y)$, where $p(x,C)$ denotes the transition probability from x into the set C. The definition is fulfilled for the Euler-Maruyama scheme applied to the SDEs investigated here. As a set A we can choose any open ball of radius 1; then (i) holds. Other choices are possible of course. As set B we can choose an arbitrary different open ball of radius 1. Let $p(x,y)$ denote the transition probability density to go from x to y. Then, as function q we can choose the constant $\inf\{p(x,y) : x \in A, y \in B\} > 0$, and as measure ρ we can choose $\rho(C) = |B \cap C|/|B|$, where $|\cdot|$ denotes the Lebesgue measure. Then (ii) holds. Here we followed example 6.2. on page 326 of [27]. The systems we consider are furthermore recurrent.
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$$\begin{aligned}
&\widehat{\Pi}^Y_k(\mathbf{x}) = \Pr(\mathbf{x}|\mathbf{x} \in Y_K) = \Pr(\mathbf{x},\mathbf{x} \in Y_k)/\Pr(\mathbf{x} \in Y_k)\\
&= \textstyle\sum_l \Pr(\mathbf{x},\mathbf{x} \in Y_k,\mathbf{x} \in Y_{kl})/\Pr(\mathbf{x} \in Y_k)\\
&= \textstyle\sum_l \Pr(\mathbf{x}|\mathbf{x} \in Y_k,\mathbf{x} \in Y_{kl})\Pr(\mathbf{x} \in Y_k,\mathbf{x} \in Y_{kl})/\Pr(\mathbf{x} \in Y_k)\\
&= \textstyle\sum_l \Pr(\mathbf{x}|\mathbf{x} \in Y_k,\mathbf{x} \in Y_{kl})\Pr(\mathbf{x} \in Y_{kl}|\mathbf{x} \in Y_k)\\
&= \textstyle\sum_l \widehat{\widehat{\Pi}}^Y_{kl}(\mathbf{x})\widehat{\Pi}^Y_k(Y_{kl}).
\end{aligned}$$

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