Flux of Particles in Sawtooth Media

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We study Brownian motion in chains of segments with flashing sawtoothlike potentials. In all former models for stochastic ratchets a coherent switching of the potential is assumed. We consider the generalized case which allows independent switchings of the potential in single segments. We introduce three different rules: correlated, anticorrelated, and uncorrelated switchings. On the basis of a discrete model analytical results for the mean flux are compared with computer simulations. As a result the mean flux will be enhanced for anticorrelated and uncorrelated sawteeth as compared with the case of correlated (coherent) segments. [S0031-9007(97)04434-7]

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Inspired by theoretical studies and biological systems the phenomenon of noise induced transport has attracted great interest in recent years [1]. To move mesoscopic particles in a certain direction by the help of unbiased fluctuations the system must have two essential features. (1) The particles move in a so-called ratchet potential U. It consists in the simplest case of a periodic sequence $U(x) = U(x + L)$ of sawtoothlike segments. It is essentially that within each segment the reflection symmetry is broken $[U(x + L/2) \neq U(-x + L/2); x \in (0, L/2)]$. (2) The system is driven out of equilibrium [2]. This requires the action of, e.g., external colored noise [1,3–5] or non-Gaussian white noise [6].

The combination of both features causes a violation of the principle of detailed balance. This gives rise to an effective transport of particles in a certain direction [2,7–12].

Mainly two different types of ratchet devices have been previously discussed [13,14]. The first class is formed by systems where external nonequilibrium forces with zero mean act [1,3,5,6,9,15–17]. These are termed changing force ratchets and provide an interesting idea for separation devices, because the particle flux may change direction for certain noise parameters [3,9,18]. The second type groups systems with a fluctuating potential profile $U(x, \sigma(t))$ [2,4,7,8,10,13]. These are termed flashing ratchets (FR) and have been discussed in connection with motor proteins. The simplest case is a simultaneous dichotomic modulation of the potential $U(x, \sigma(t)) = (1/2)[1 + \sigma(t)]U(x)$ with $\sigma(t) = \pm 1$. The whole chain of the N sawteethlike segments adopts two states: $U(x, \sigma = 1) = U(x)$, and $U(x, \sigma = -1) = 0$. A particle which is first localized in a minimum of the sawtooth potential will diffuse freely after the potential is switched "off." If the asymmetric potential is turned "on" again the expanded probability density of the particle will be cut at different distances to the left and to the right from the original minimum. This yields an effective particle flux in a certain direction.

As described above in previous works on FR and motor proteins [2,4,7,8,10] the sawtooth potential in all N segments of the chain is switched simultaneously on and off. This assumption of coherent switching of all sawteeth can be reduced mathematically to a single segment with periodic boundary conditions. We will call this the correlated switching rule, later on. If the potential $U(x)$ is replaced by $-U(x)$ the mean flux changes the sign, but its absolute value is invariant.

The main point of this Letter is to introduce local rules for the switching of the potential in every segment. The independent switching of neighboring segments is modeled by the assignment of a random number $\sigma_i = \pm 1$ to every segment $i = 1, 2, \ldots, N$, indicating its instantaneous switching state (Fig. 1). We will assume that the flashing of a single sawtooth i follows from a dichotomic Markov process, which flips between $\sigma_i = 1$ and $\sigma_i = -1$ with a probability γ per unit time.

We will restrict ourselves to three different rules which can be distinguished by the two point correlation function $\langle \sigma_{i+1} \sigma_i \rangle$:

(a) Correlated: $\sigma_{i+1} = \sigma_i$ ($\langle \sigma_{i+1} \sigma_i \rangle = 1$).
(b) Anticorrelated: $\sigma_{i+1} = -\sigma_i$ ($\langle \sigma_{i+1} \sigma_i \rangle = -1$).
(c) Uncorrelated: $\langle \sigma_{i+1} \sigma_i \rangle = 0$.

The angular brackets denote averaging over the dichotomous noise. Case (a) corresponds to the coherent switching of all segments as formerly discussed. In the anticorrelated case (b) again the chain adopts two states only. The potential has a period of two segments. If in the first state, e.g., every segment with an odd index i is switched on, the neighbors with even numbers are off.

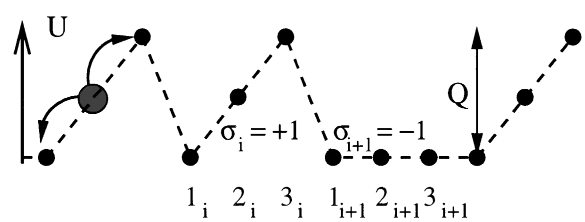

FIG. 1. In the uncorrelated ratchet every sawtooth i switches on ($\sigma_i = +1$) and off ($\sigma_i = -1$) independently of its neighbors. The points should hint schematically at the three energy levels of the discrete model.

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Respectively, in the second state the even segments are on and the odd ones off. Compared with former investigations a qualitatively new situation is the uncorrelated case (c). The switching of each segment is independent from its adjacent segments. The number of possible configurations $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ for this uncorrelated chain with N segments is 2^N.

We will calculate analytically the mean flux of particles for all three situations and support our results by computer simulations. The flux is maximum for the anticorrelated case. Also for the uncorrelated chain we find an enhanced mean flux compared to the correlated case using a mean field approximation. Surprisingly, the symmetry of the current with respect to the change of the sign of the potential is broken in the cases (b) and (c).

For a single sawtooth segment i we use an analytically solvable model of a FR consisting of discrete steps (Figs. 1 and 2). The spatial movement of a particle is modeled as a random walk with jumps $n \rightarrow n \pm 1$. Broken reflection symmetry requires at least three discrete steps per sawtooth. Jumps involving the "inner" state $n = 2$ occur with a rate $W(n \rightarrow n \pm 1, \sigma_i)$. It depends on the switching state σ_i of the instantaneous occupied segment i. The states $n = 1$ and $n = 3$ are border points between different segments i and $i \pm 1$. Hence, it is implied that the state $n = 4$ forms state $n = 1$ of the following segment, and $n = 0$, respectively, state $n = 3$ of the segment to the left. So in the following we will use n in the sense of $n \, mod \, 3$. We declare that the previous segment defines the transition rates between adjacent neighbors. Jumps between $n = 3$ and $n = 1$ occur with $W(n \rightarrow n \pm 1, \sigma_{i-1})$.

A definition of the forward transition probabilities, by using a Arrhenius-like expression simply reads

$$W(n \rightarrow n + 1, \sigma_i(t)) = a e^{-\Delta U(n)[\sigma_i(t)+1]/2k_BT}. \quad (1)$$

Here $\Delta U(n)$ denotes the difference of the energy levels in the states n and $n + 1$. In (1) the Boltzmann number is denoted by k_B and T is the absolute temperature. Correspondence to particle motion in a piecewise linear sawtooth potential is obtained by choosing $\Delta U(n) = Q/2$ for $n = 1, 2$ and $\Delta U(3) = -Q$. Backward transitions have reciprocal rates: $W(n + 1 \rightarrow n, \sigma_i(t)) = 1/W(n \rightarrow n + 1, \sigma_i(t))$ excluding $n = 1$ which by definition depends on the state of the predecessor $W(1 \rightarrow 3) = 1/W(3 \rightarrow 1, \sigma_{i-1})$.

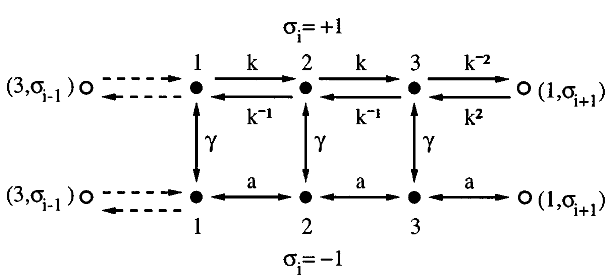

FIG. 2. In the discrete ratchet model one segment consists of three spatial states $n = 1, 2, 3$ and two switching states σ. A suitable choice of the boundaries allows the investigation of chains with arbitrary length.

This picture is simplified by introducing the abbreviation $k = \exp(-Q/4k_BT)$. In the on state forward jumps occur per unit time from $n = 1, 2$ with rate k and from $n = 3$ with k^{-2}. The on state $\sigma_i = 1$ corresponds to a random walk in the potential $U(n)$. In the off state $\sigma = -1$ the walker simply performs random motion with equal rates between all states $W(n \rightarrow n \pm 1, -) = a$. For simplicity we will set $a = 1$, later on.

The consideration of a chain with N sawteeth can be reduced to the analysis of a single segment with given adjacent states. Let $P(n, \sigma_i, \bar{\sigma}_i, t)$ be the probability of finding the system in the state (n, σ_i) at time t with given $\bar{\sigma}_i = (\sigma_{i-1}, \sigma_{i+1})$. This probability function obeys the master equation:

$$\partial_t P(n, \sigma_i, \bar{\sigma}_i, t) = \Delta J(n, \sigma_i, \bar{\sigma}_i) - \gamma P(n, \sigma_i, \bar{\sigma}_i, t) + \gamma P(n, -\sigma_i, \bar{\sigma}, t), \quad (2)$$

where $\Delta J(n, \sigma_i, \bar{\sigma}_i)$ arises from the difference of probability fluxes for given values of $\sigma_i, \bar{\sigma}_i$. The second part in (2) describes the switching $\sigma_i \rightarrow -\sigma_i$.

The fluxes involving the internal state $n = 2$ depend only implicitly on the states of the adjacent segments. It follows simply

$$\Delta J(2, \sigma_i, \bar{\sigma}_i) = J(1, \sigma_i, \bar{\sigma}_i) - J(2, \sigma_i, \bar{\sigma}_i), \quad (3)$$

where $J(n, \sigma_i, \bar{\sigma}_i)$ is the flux between n and $n + 1$

$$J(n, \sigma_i, \bar{\sigma}_i) = W(n \rightarrow n + 1, \sigma_i) P(n, \sigma_i, \bar{\sigma}_i) - W(n + 1 \rightarrow n, \sigma_i) \times P(n + 1, \sigma_i, \bar{\sigma}_i). \quad (4)$$

The fluxes involving the border states $n = 1, 3$ are determined by the fluxes from the internal state and, additionally, by fluxes across the border to the adjacent segments. We denote the flux from the left between the segment i and its predecessor $i - 1$ pointing inside the ith segment by $J(\sigma_{i-1}, \sigma_i)$. It reads

$$J(\sigma_{i-1}, \sigma_i) = W(3 \rightarrow 1, \sigma_{i-1}) P(3, \sigma_{i-1}, \bar{\sigma}_{i-1}) - W(1 \rightarrow 3, \sigma_{i-1}) P(1, \sigma_i, \bar{\sigma}_i). \quad (5)$$

This expression takes into account that the transition rate to the neighbor is determined by the switching state σ_{i-1} of the left predecessor. Here $J(\sigma_i, \sigma_{i+1})$ stands for the current on the right border, pointing outside.

Hence for the left border state $n = 1$

$$\Delta J(1, \sigma_i, \bar{\sigma}_i) = J(\sigma_{i-1}, \sigma_i) - J(1, \sigma_i, \bar{\sigma}_i) \quad (6)$$

and for $n = 3$, respectively,

$$\Delta J(3, \sigma_i, \bar{\sigma}_i) = J(2, \sigma_i, \bar{\sigma}_i) - J(\sigma_i, \sigma_{i+1}). \quad (7)$$

In the following we will solve Eq. (2) in the long time limit $\partial_t P^0(n, \sigma_i, \bar{\sigma}_i) = 0$. The stationary state with violated detailed balance implies constant currents through the segments $J^0 = \sum_{\sigma_i,\bar{\sigma}_i} J(n, \sigma_i)$ for all n. From (6) and (7) it immediately follows that $J^0 = \sum_{\sigma_i,\bar{\sigma}_i} J(\sigma_{i-1}, \sigma_i) = \sum_{\sigma_i,\bar{\sigma}_i} J(\sigma_i, \sigma_{i+1})$. Different switching rules will imply the formulation of special closure conditions. In result Eq. (2) in all three cases will reduce to six coupled linear algebraic equations plus the normalization condition which can be solved.

First we consider the correlated case $\sigma_i = \sigma_{i\pm1}$. Assuming periodicity of the solution $P^0(n, \sigma_{i\pm1}, \bar{\sigma}_{i\pm1}) = P^0(n, \sigma_i, \bar{\sigma}_i)$ implies that the fluxes between adjacent segments are adjusted so that $J(\sigma_{i-1}, \sigma_i) = J(\sigma_i, \sigma_{i+1}) = J(\sigma_i, \sigma_i)$. This means that in (5) σ_{i-1} has to be replaced by σ_i.

We will not present here the rather long algebraic expression. The stationary flux J^0 versus the switching rate γ is plotted for $k = 0.2$ in Fig. 3. Additionally we compare with numerical simulations of our discrete model, which were carried out using Gillespie's algorithm [19]. In qualitative agreement with the results [2,4,10] for a spatially continuous flashing ratchet we find a maximal flux for a suitable value γ. For fast switching the system cannot adjust to the asymmetry of the jump rates, so the current vanishes for $\gamma \to \infty$. In the absence of switching ($\gamma = 0$) the system decomposes into two independent components. For both σ_i the states n are occupied with the Boltzmann probability $P(n, \sigma_i) \sim \exp[-U(n, \sigma_i)/k_B T]$ and the detailed balance is obeyed. The fluxes J for both values of σ_i vanish. The location of the maximal current grows monotonically with decreasing k. The absolute value of the flux approaches a maximum for $\gamma \approx 2.3$ and $k \approx 0.2$. Changing the sign of the potential or replacing k by k^{-1} would reverse the flux with the same absolute value (Fig. 4).

The closure condition found for the anticorrelated ratchet $\sigma_{i-1} = -\sigma_i = \sigma_{i+1}$ leads to $J(\sigma_{i-1}, \sigma_i) = J(-\sigma_i, \sigma_i)$ and $J(\sigma_i, \sigma_{i+1}) = J(\sigma_i, -\sigma_i)$. For the uncorrelated ratchet the exact formulation of similar symmetry relations is not possible. For a given σ_i the potential states $\sigma_{i\pm1}$ of the neighboring sawteeth are random numbers and the fluxes across the borders $J(\sigma_{i-1}, \sigma_i)$ and $J(-\sigma_i, \sigma_{i+1})$ are random as well. Hence, dependent on the actual adjacent state we have

$$J(\sigma_{i-1}, \sigma_i) = \frac{1}{2}(1 + \sigma_{i-1}\sigma_i)J(\sigma_i, \sigma_i) + \frac{1}{2}(1 - \sigma_{i-1}\sigma_i)J(-\sigma_i, \sigma_i) \quad (8)$$

and, respectively,

$$J(\sigma_i, \sigma_{i+1}) = \frac{1}{2}(1 + \sigma_i\sigma_{i+1})J(\sigma_i, \sigma_i) + \frac{1}{2}(1 - \sigma_i\sigma_{i+1})J(\sigma_i, -\sigma_i). \quad (9)$$

Expressions (8) and (9) are valid for all switching rules. In the uncorrelated case we make use of a mean field approximation and replace the actual values $\sigma_{i-1}\sigma_i$ by $\langle\sigma_{i-1}\sigma_i\rangle = 0$

In Fig. 3 the fluxes of the three cases are depicted for a given value of $k = 0.2$. The flux for uncorrelated and anticorrelated situations, compared to the usually considered correlated case, is enhanced for all switching rates γ. This remains valid qualitatively for all relevant values $0 < k < 1$. The higher flux is caused by the following: In the correlated case a diffusive transport of a particle between different segments takes place in the off case only. The particle has to stay at least the time $\tau = \gamma^{-1}$ of the on state within one segment. The transport is interrupted. On the contrary, in the other cases an effective transport might take place at all times.

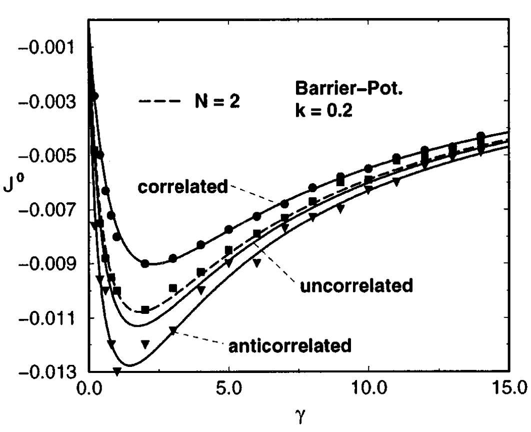

FIG. 3. Current J vs switching rate γ ($k = 0.2$) for correlated, uncorrelated, and anticorrelated ratchets (from top to bottom). The lines are the analytical calculations described in the text, while the points are obtained by computer simulations ($N = 10$). The mean field result for the uncorrelated ratchet deviates from the exact solution in the case $N = 2$ (dashed line).

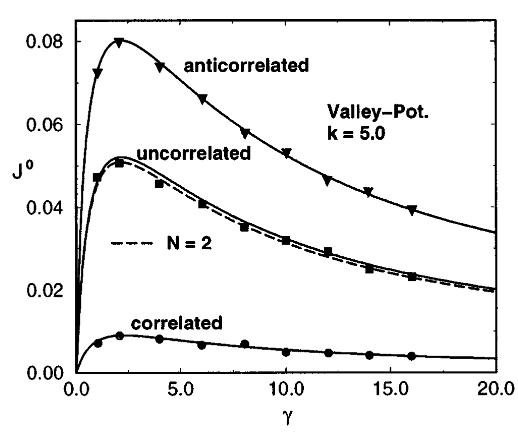

FIG. 4. Current J vs switching rate γ for valley potentials ($k = 5.0$) and anticorrelated, uncorrelated, and correlated switching (from top to bottom). The symbols show computer simulations for $N = 10$ and the lines are analytical calculations. The dashed line shows the exact solution for uncorrelated switching in the case $N = 2$, which deviates from the mean field approximation.

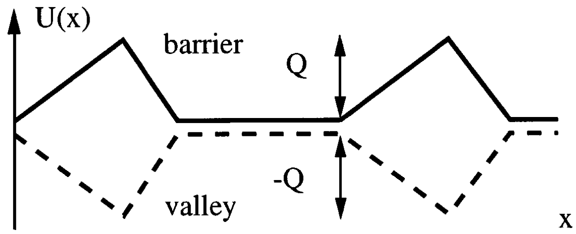

FIG. 5. The inversion of the anticorrelated potential leads to a valley potential.

During two switching times τ the particle is able to reach the next but one segment.

A more drastic change of the particle flux is observed, if the sign of the potential is changed $[U(x) \rightarrow -U(x)]$ or, equivalently, by the replacement $k \rightarrow k^{-1}$. The results are plotted in Fig. 4. While in the correlated situation the direction of the current changes only, the uncorrelated and anticorrelated chains strongly enhance the absolute value of the flux (the latter nearly by 1 order of magnitude). This is shown in Fig. 4 for $k = 5.0$, but we tested the effect of flux enhancement for $1 < k \leq 10^5$. This behavior is caused by the shape of the potential as illustrated in Fig. 5 for an anticorrelated ratchet. While in the original ($U > 0$) the areas of constant plateaus (no force) are embedded by repelling segments, in the image ($U < 0$) they are surrounded by attracting forces. We call this barrier ($k < 1$) and valley potentials ($k > 1$).

The results were verified by computer simulations of ratchets with $N = 10$, 30, and 50. We found no dependence on the chain length N. For instance, the results for $N = 10$ are included in Figs. 3 and 4. Furthermore we solved Eq. (2) for the special case $N = 2$. For the uncorrelated segments periodic boundary conditions over $2L$ were assumed. For the correlated and anticorrelated ratchet the solution agrees with the above described results. In case of the uncorrelated switching rule we found a discrepancy between the mean field approximation and the special solution for two segments. The calculated fluxes differ for all relevant parameter values by maximally 8%. In comparison with the simulations the mean field description overestimates the absolute value of the current.

In conclusion we have presented distributed models, which enhance the particle flux in FRs. For valley potentials with anticorrelated switching (b) of adjacent neighbors a maximum current was found. Since such behavior was observed for large parameter ranges, this suggests a new possibility for the construction of high efficient Brownian motors. Suitable ratchet devices could be realized by electrical fields [7] using separately controllable electrodes. By comparison with biological data [4] we find that the effect of flux amplification is most important in systems on the length scale of 10 nm with switching times of the order 10^{-4} s and energy barriers of $10k_BT$. The uncorrelated rule (c) enables further insight into transport mechanisms in stochastic ratchets. The proposed flux description of many segments is generalizable to different potential shapes. In particular a two dimensional extension of our model should be possible, where every sawtooth is taken as an input-output element [20].

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