

Multiple current reversal in Brownian ratchets

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We address the problem of stationary transport of overdamped Brownian particles in a one-dimensional spatially periodic potential composed of N hills within one period. We show that in a system driven by both thermal equilibrium fluctuations and symmetric dichotomic fluctuations, a proper manipulation of the barrier heights and slopes of the potential leads to multiple drift velocity reversal. Under optimal conditions, the drift velocity as a function of temperature and intensity of dichotomic fluctuations possesses as many as N extrema of alternating signs. There exist $N-1$ values of a critical temperature which separate regimes of opposite directions of particle transport.

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I. INTRODUCTION

Transport phenomena play a crucial role in a large variety of processes in nature, from physical through biological to social systems. In the past ten years or so, the concept of stochastic transport realized in Brownian ratchets has captured the attention of researchers [1]. Ratchets are one example of simple nonequilibrium model systems which, in the absence of any bias forces and gradients, can rectify zero-mean nonequilibrium fluctuations into unidirectional motion. Various ratchetlike mechanisms have been intensively studied, including an analysis of sources of driven (deterministic and/or random) forces or potentials, statistics of nonthermal fluctuations, conditions for optimal transport, etc., [2]. The subject has become attractive for at least two reasons: the possibility of a satisfactory explanation of directed motion of molecular motors which transport macromolecules in biological cells [3], and attempts to construct well-controlled devices of high resolution for separation of macro-particles and microparticles like cells, latex spheres, DNA, or proteins [4]. In both cases the magnitude and direction of the drift velocity of particles are important characteristics of transport. In this context, the current reversal phenomenon is one of the most interesting aspects of the theory of Brownian ratchets.

In this paper we study a system which exhibits multiple current reversal. We show that the right deformation of shape of the spatially periodic potential can almost arbitrarily change the qualitative features and properties of the system. In real systems the shape of the potential is a feature which can be changed or adjusted. In biological systems, the potential is related to the size, shape, and components of proteins, which in general are very complicated, and the potential is reckoned to be highly fine tuned by biological evolution. Protofilaments, which form a microtubulin, are one-dimensional spatially periodic systems consisting of an α tubulin and β tubulin, which influence transport of kinesin or dynein along microtubulins. In separation devices the shape of the potential can be obtained, e.g., by microlithographic techniques, and they can be quite complex.

The remainder of this paper is organized as follows. In Sec. II we describe the mathematical model of the thermal

ratchet under study. It is a model with a fluctuating force; exponentially correlated symmetric two-state Markov noise. This is one of the simplest correlated noises which can induce transport in periodic structures with broken reflection symmetry. A Brownian ratchet with this driving was already investigated in the literature [5–8]. In Ref. [6] it was shown that asymmetric dichotomic noise and a simple piecewise linear potential can produce a current reversal. Its origin comes from the interplay between the asymmetry of the periodic potential and the asymmetry of the noise. Here we do not adopt this mechanism: the noise considered is symmetric. However, potentials are asymmetric and much more complicated. In Sec. III we construct such potentials, which consist of N hills within one period. For simplicity, we have considered piecewise linear functions. In Sec. IV we show that the ratchet system exhibits a multiple current reversal which is generated by the potentials constructed in Sec. III.

II. MODEL

We analyze the stochastic dynamics of overdamped and noninteracting Brownian particles moving in a one-dimensional spatially periodic potential $\hat{V}(\hat{x}) = \hat{V}(\hat{x} + L)$ of period L and of the maximal barrier height $\Delta\hat{V} = \hat{V}_{max} - \hat{V}_{min}$, and driven by two random forces. The Langevin equation of motion in dimensionless form is (the scaling and dimensionless variables were discussed in detail in Ref. [9])

$$\dot{x} = f(x) + \Gamma(t) + \xi(t), \quad f(x) = -dV(x)/dx, \quad (1)$$

where $x = \hat{x}/L$ is a dimensionless position of the Brownian particle, and $V(x) = V(x+1)$ is a rescaled periodic potential with a unit period and a unit maximal barrier height. The random force $\Gamma(t)$ represents equilibrium thermal fluctuations. It is Gaussian white noise of zero average, $\langle \Gamma(t) \rangle = 0$, and the correlation function $\langle \Gamma(t)\Gamma(s) \rangle = 2D\delta(t-s)$, where $D = k_B T / \Delta\hat{V}$ is its intensity, k_B stands for the Boltzmann constant, and T is the temperature of the system. The random force $\xi(t)$ represents nonequilibrium fluctuations, and is modeled by a *symmetric* dichotomic Markovian stochastic process,

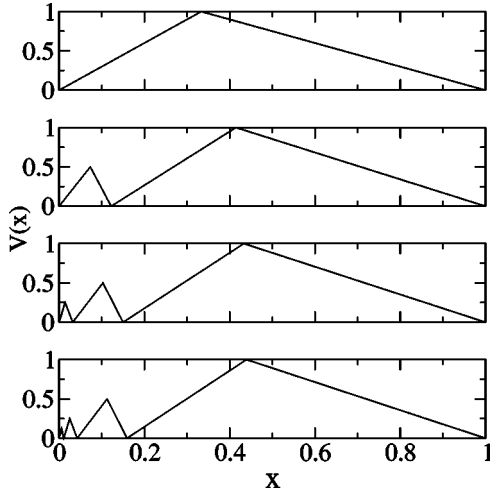


FIG. 1. The rescaled sawtooth potentials of unit period and unit maximal barrier height within one period with $N=1, 2, 3$, and 4 hills (top to bottom). The values of barrier-heights and slopes are given in Eq. (11).

$$\xi(t) = \{-a, a\}, \quad a > 0, \quad (2)$$

$$P(-a \rightarrow a) = P(a \rightarrow -a) = \mu,$$

where $P(-a \rightarrow a)$ is a probability per unit time of the jump from state $-a$ to state a . This process is of zero average, $\langle \xi(t) \rangle = 0$, and exponentially correlated,

$$\langle \xi(t) \xi(s) \rangle = a^2 e^{-|t-s|/\tau}, \quad (3)$$

where $\tau = 1/2\mu$ is the correlation time of the process $\xi(t)$. Thus, it is characterized by two parameters: its amplitude a (or equivalently the variance $\langle \xi^2(t) \rangle = a^2$) and the correlation time τ .

Master equations corresponding to Eq. (1) have the forms [10]

$$\frac{\partial P_+(x,t)}{\partial t} = -\frac{\partial}{\partial x}[f(x)+a]P_+(x,t) + D \frac{\partial^2}{\partial x^2} P_+(x,t) - \mu P_+(x,t) + \mu P_-(x,t), \quad (4)$$

$$\frac{\partial P_-(x,t)}{\partial t} = -\frac{\partial}{\partial x}[f(x)-a]P_-(x,t) + D \frac{\partial^2}{\partial x^2} P_-(x,t) + \mu P_+(x,t) - \mu P_-(x,t), \quad (5)$$

where the probability densities are

$$P_+(x,t) \equiv p(x, a, t), \quad P_-(x,t) \equiv p(x, -a, t). \quad (6)$$

From Eqs. (4) and (5) it follows that the probability density

$$P(x,t) = P_+(x,t) + P_-(x,t) \quad (7)$$

of the process $x(t)$ alone obeys the continuity equation

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}, \quad (8)$$

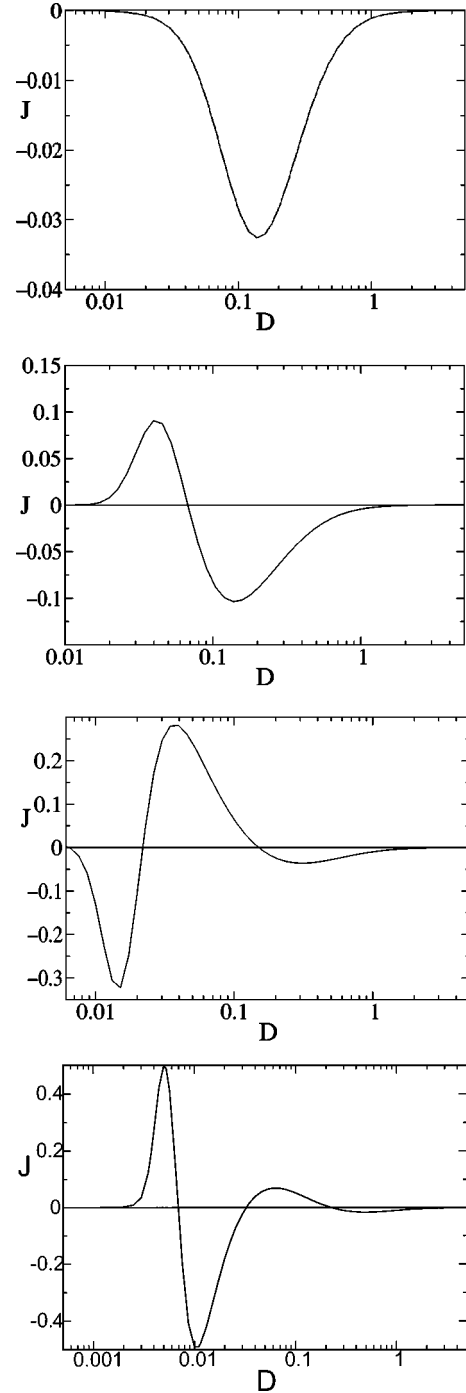


FIG. 2. The dimensionless current vs dimensionless intensity D of thermal fluctuations (or temperature of the system) for potentials (11) with 1, 2, 3, and 4 hills. Values of the amplitude a of dichotomic fluctuations are $a=1.8$ for $N=1$, $a=4.78$ for $N=2$, $a=10.58$ for $N=3$, and $a=16.7$ for $N=4$. The correlation time of dichotomic noise is $\tau=1.0$.

where the probability current

$$J(x,t) = f(x)P(x,t) - D \frac{\partial P(x,t)}{\partial x} + a[P_+(x,t) - P_-(x,t)]. \quad (9)$$

This is a fundamental quantity characterizing transport properties of the system. In particular, the averaged drift (dimensionless) velocity $v(t)$ of the particles is given by the relation

$$v(t) = \langle \dot{x} \rangle = \int_0^1 f(x) P(x, t) dx = \int_0^1 J(x, t) dx, \quad (10)$$

and the latter follows from the former by use of Eq. (9).

III. POTENTIALS

If nonequilibrium fluctuations $\xi(t)$ are symmetric [11], transport and directed motion of particles is possible only when the spatial reflection symmetry of the potential $V(x)$ is broken. If $V(x)$ is a simple piecewise linear function having one maximum within a period (a generic ratchet potential used in literature), the current reversal phenomenon can occur only when fluctuations are asymmetric [11]. In the case of symmetric fluctuations $\xi(t)$, this phenomenon can occur if the shape of the potential is deformed in a special way [12]. We show this by analyzing a case of a potential which is composed of N hills of various heights and shapes. For the sake of simplicity, piecewise linear potentials on the unit interval $[0, 1]$ will be considered, assuming that their minimal values are zero and $V(0) = V(1) = 0$. We define a sawtooth potential by fixing two independent sets of numbers: its maximal values $V = [V_1, V_2, \dots, V_N]$ and values of the slope (force) $f = [f_1^-, f_1^+, f_2^-, f_2^+, \dots, f_N^-, f_N^+]$. Hence the triple $[V_i, f_i^-, f_i^+]$ characterizes the i th tooth of the potential. We expect that, by appropriate manipulation of its heights and slopes, the N -sawtooth potential gives rise to the multiple current reversal. This conjecture follows from two observations. First, if $\xi(t) = 0$ the motion of a Brownian particle in a potential with hills of various heights consists of subsequent barrier crossings in one of three regimes:

- (i) $V_i \ll D$; the motion of the particle is not essentially disturbed by the barrier, and is of diffusive type.
- (ii) $V_i \approx D$; the motion of the particle is of activation type.
- (iii) $V_i \gg D$; the long-distance motion of the particle is not possible without driving force (here by dichotomic fluctuations).

Second, at zero temperature the barrier crossing induced by dichotomic noise only depends on the relation between the slopes and the amplitude a of fluctuations $\xi(t)$. Taking the above into account, we construct potentials fulfilling the following conditions:

- (a) Potentials have increasing barriers: $V_i < V_{i+1}$.
- (b) The smaller barrier has steeper slopes than slopes of all higher barriers, i.e., if $V_i < V_k$ then $|f_i^-|, |f_i^+| > |f_k^-|, |f_k^+|$.
- (c) Barriers have alternating asymmetry, i.e., if $|f_i^-| > |f_i^+|$ (or vice versa) then $|f_{i+1}^-| < |f_{i+1}^+|$ (or vice versa).

As an example, we analyze four cases of the following potentials (see Fig. 1)

$$N=1: \quad V=[1], \quad f=[3, -1.5], \quad (11)$$

$$N=2: \quad V=[0.5, 1], \quad f=[6.83, -10.25, 3.42, -1.71],$$

$$N=3: \quad V=[0.25, 0.5, 1],$$

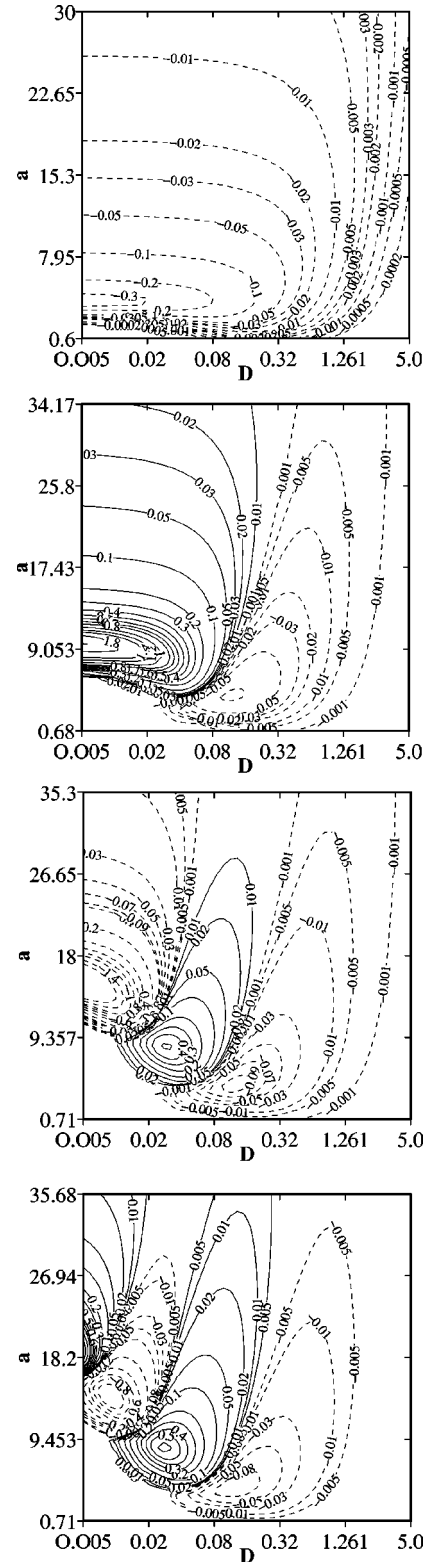


FIG. 3. The dimensionless current vs dimensionless intensities of dichotomic and thermal fluctuations for the potentials (11) with 1, 2, 3, and 4 hills. Dashed and solid lines denote negative and positive values of the current, respectively. The correlation time of dichotomic noise is $\tau = 1.0$. The scale of D is logarithmic, and the scale of a is linear.

$$f = [17.65, -14.12, 7.06, -10.59, 3.53, -1.77]$$

$$N=4: \quad V = [0.125, 0.25, 0.5, 1],$$

$$f = [21.41, -24.98, 17.84, -14.27, 7.14, -10.70, 3.57, -1.78].$$

IV. RESULTS

We consider a stationary regime in which the probability density $P(x) = \lim_{t \rightarrow \infty} P(x, t)$, and the probability current $J = \lim_{t \rightarrow \infty} J(x, t) = \text{const}$. The stationary mean (dimensionless) velocity v of the particle is equivalent to the current J :

$$v = \langle \dot{x} \rangle = \int_0^1 f(x) P(x) dx = J. \quad (12)$$

The stationary probability current can be obtained from Eq. (9), and takes the form

$$J = f(x)P(x) - DP'(x) + a[P_+(x) - P_-(x)], \quad (13)$$

where the prime denotes a derivative with respect to x .

For an arbitrary potential, the stationary solution of the system of equations (4) and (5) is not known, with the exception of some limiting cases. For a piecewise linear potential this system can be solved analytically. The method of solution was presented in Ref. [10] for the simplest piecewise linear potential with $N=1$ hill. Though this potential is very simple, the calculations require an algebra manipulation package, and the final analytical results have to be investigated numerically due to their complexity, illegibility, and length. Here, in order to obtain reliable results, we have decided to obtain numerically a stationary solution $\{P_+(x), P_-(x)\}$ of the system of equations (4) and (5). For this purpose we have adapted the finite elements method. Next, the stationary current J is obtained from relation (13). In practice, this allows one to obtain the solution in the shorter CPU time and of the same accuracy as the analytical approach. Moreover, it is much easier to implement this method for an arbitrary form of the potential $V(x)$.

A general note concerns the dependence of the current on the correlation time τ of dichotomic noise. In the fast noise limit, when $\tau \rightarrow 0$, the current diminishes: $J \rightarrow 0$. For small τ it behaves as $J \propto \tau^\alpha$. The value of the exponent α depends strongly on the regularity of the potential $V(x)$. Its value has been evaluated for a smooth potential [7] as well as for a piecewise linear potential with $N=1$ hill [8]. For an arbitrary N , this problem has not been studied. In the slow noise limit, when $\tau \rightarrow \infty$, the system of equations (4) and (5) decouples, and then $J \rightarrow J_\infty$, where

$$J_\infty = [J(a) + J(-a)]/2 \quad (14)$$

and

$$J(a) = D \frac{1 - e^{-a/D}}{\int_0^1 e^{-(V(x)-ax)/D} \int_x^{x+1} e^{(V(y)-ay)/D} dy dx}. \quad (15)$$

From a numerical analysis it follows that for any N the current $J(\tau)$ as a function of the correlation time τ can change sign at most once, i.e., there is such a value of $\tau = \tau_i$ that $J(\tau_i) = 0$. Below τ_i and above τ_i particles are transported in opposite directions. On the other hand, for fixed N there exists such a domain of values of the amplitude a and correlation time τ of fluctuations $\xi(t)$ that the current $J(D)$ as a function of the thermal noise intensity D (i.e., temperature) possesses N extrema of alternating signs. As a consequence, $J(D) = 0$ for $N-1$ values of $D = D_1, D_2, \dots, D_{N-1} > 0$ (see Fig. 2). In each, two adjacent domains separated by D_i particles move in opposite directions. We have observed that if N becomes greater and greater then extrema of J for higher temperatures are smaller and smaller. Of course, this is only true for potentials constructed in such a way as presented in Sec. III. In Fig. 3 we present a contourplot of the current as a function of the thermal-noise intensity D and the amplitude a of the dichotomic noise. One can see that, for fixed D and a correlation time τ , a multiple current reversal occurs when a is varied.

The multiple current reversal can be detected for slow fluctuations as well. Indeed, from numerical analysis of formula (14), we have qualitatively obtained the same behavior of the current as presented in Fig. 2. We have investigated the dependence of the original unscaled (dimensional) mean velocity $\langle v \rangle = (\Delta \hat{V} / \gamma L) J$ of particles on their linear size R , which, via the Stokes formula, is hidden in the friction coefficient $\gamma \propto R$. The detailed procedure was described in Ref. [10]. We have noted that the mean velocity can change its sign only once when R is changed monotonically and, unfortunately, multiple velocity reversal is not possible in this case.

In conclusion, we have shown that in a system driven by symmetric fluctuations and noise, the phenomenon of multiple current reversal can be precisely controlled by the proper deformation of a spatially periodic potential. This phenomenon occurs upon variation of not all but only selected basic parameters of the model (here by the thermal-noise intensity D and the amplitude of the nonthermal noise a). Multiple current reversal can appear in other systems [13,14]. However, the mechanism is radically different than that studied in this paper.

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