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Current of loaded particle in two-dimensional tube with varying width

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ABSTRACT

The current of a loaded particle along a two-dimensional (2D) tube with non-straight midline and is investigated. It is found that in the case of a load with an asymmetric unbiased external force, the limits of temperature and asymmetric external force for particle directed moving become smaller as the load increased. The directed current is a peaked function of temperature and amplitude of the asymmetric unbiased external force. As the channel width is decreased, the directed current decreases with the increase of the load.

1. Introduction

The problem of particles transport in narrow, tortuous confining structures has been extensively studied due to its important in many fundamental processes, i.e., molecules passing through ion channel proteins, molecular sieves and molecular motors moving along internal organelles [1,2]. A key point in understanding the nature of these processes is that the shape of the tube and the boundary effects play a nontrivial role. Most studies regarded the geometric constraints and boundary effects as entropic barriers and reduced the dimensionality of the problem via the Fick–Jacobs (FJ) approximation [2–5]. Based on an asymptotic expansion in a small dimensionless parameter that characterizes the channel width, Bradley [6] proved the validity of the FJ equation to zeroth order in the small dimensionless parameter and found it can be taken on the same form for both symmetric and asymmetric channels. Using the FJ equation, Reguera [7] studied a Brownian particle moving in asymmetric channel with a biased external force in presence of entropic barriers. They found that temperature dictates the strength of the entropic potential, and thus an increase in temperature leads to a reduction of the current. Ai [8–10] investigated the transport of Brownian particles with entropic barriers and an unbiased external force. They found that the asymmetry of the tube shape and the asymmetry of the unbiased forces are the two ways of inducing a net current, and the phase shift between the entirely symmetric tube and noise modulation can break the symmetry of the generalized potential and induce directed transport. In their later work [11], they studied Brownian particles transport in deformable tube and found that the competition between the deformation and the asymmetric driving forces will induce rich phenomena in transport, i.e., the current can be enhanced by choosing appropriate noise intensity and deformation. Recently, from the combination of transient transport mechanisms and asymmetric channel geometry, Alvarez-Ramirez [12] explained the Brownian particles transport asymmetry and found that for certain channel configurations, Brownian particles are preferentially transported in one axial direction (e.g., left-to-right) than in the opposite axial direction.

Most studies about the particle transport and load force induced by non-equilibrium fluctuations have relied on the energy barrier [13–16], only few studies [8,17] have considered the load effect on particles transport in presence of entropic barriers. However, in the real transport process, the particles transport with a load is also popular, such as, kinesis and dynein's move along tubulin filaments, myosin moves along action filaments [18]. When a Brownian particle works against a load, the directed current in the presence of entropic barriers exhibits peculiar behavior. Xie [17] investigated the transporting velocity of a loaded Brownian motor with entropic barrier in the presence of an asymmetric unbiased force and found that in the presence of the entropic barrier, a definite fluctuation can facilitate the loaded Brownian motor moving. This is important for designing and controlling these systems.

In this Letter, we focus on the load effects on the directed current of particle transport in a 2D tube in presence of entropic barriers. We emphasize on finding the limited scopes of temperature, amplitudes of the asymmetric external force and degrees of the

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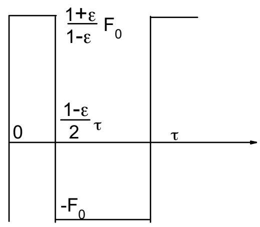

Figure 1. The schematic diagram of the asymmetric unbiased external force. τ is the period, F_0 is the amplitude, and ε is the temporal asymmetric parameter.

tube change for Brownian motor directed moving. It is expected to provide guidance to design and control the micro fluidic devices with excellent performances.

2. Model and methods

Consider a Brownian particle with a load f moving in a 2D periodic tube in the presence of an asymmetric unbiased external force (Figure 1), the corresponding stochastic dynamics of the particle under over-damped condition is described by following 2D Langevin equations in a dimensionless form [9,17]:

$$\gamma \frac{dx}{dt} = F(t) - f + \xi_x(t), \tag{1}$$

$$\gamma \frac{dy}{dt} = \xi_y(t). \tag{2}$$

where $\xi_i(t)$ are the uncorrelated Gaussian white noises with zero mean and correlation function, $\langle \xi_i(t)\xi_j(t) \rangle = 2\gamma k_B T \delta_{ij}\delta(t-t')$ for i, $j = x$, y. k_B is the Boltzmann constant and T is the absolute temperature, $\langle \ldots \rangle$ denotes an ensemble average over the distribution of noise. $\delta(t)$ is the Diracdelta function. x, y are the 2D coordinates, γ is the friction coefficient of the particle, and $F(t)$ is a temporally asymmetric unbiased external force along the x direction and satisfies:

$$F(t) = \begin{cases} \dfrac{1+\varepsilon}{1-\varepsilon}F_0, & n\tau \le t < n\tau + \dfrac{1}{2}\tau(1-\varepsilon) \\ -F_0, & n\tau + \dfrac{1}{2}\tau(1-\varepsilon) < t < (n+1)\tau \end{cases} \tag{3}$$

where τ is the period of the unbiased force, F_0 is its magnitude, ε is the temporally asymmetric parameter with $0 \le \varepsilon < 1$ which is different from the one in Refs. [9,17] because of a load.

The shape of the tube is described by its wall functions $\omega_-(x)$ and $\omega_+(x)$. The bottom wall $\omega_-(x)$ and top wall $\omega_+(x)$ are following, respectively:

$$\omega_-(x) = -\left\{ a\left[1 - \sin\left[\left(\frac{2\pi x}{L}\right) + \phi\right]\right] + b \right\}, \tag{4}$$

and

$$\omega_+(x) = a\left\{1 - \sin\left[\left(\frac{2\pi x}{L}\right) + \phi\right]\right\} + b. \tag{5}$$

Here a represents the parameter that controls the slope of the tube, L is the periodicity of the tube, φ is the relative phase shift between the bottom and top walls, and b is the narrowing of the boundary function and the radius at the bottleneck is $b-a$. The shapes of the tube are shown in Figure 2 for different values of φ.

Due to the complicated boundary conditions of diffusion in irregular channels, it is very difficult to solve Eqs. (1) and (2). Following Refs. [1–5], by eliminating of the transversal y coordinate assuming fast equilibration in the transversal channel direction, and using the concept of effective diffusion coefficient and entropic barrier, the approximate Fick–Jacobs equation corresponding to Eqs. (1) and (2) is obtained:

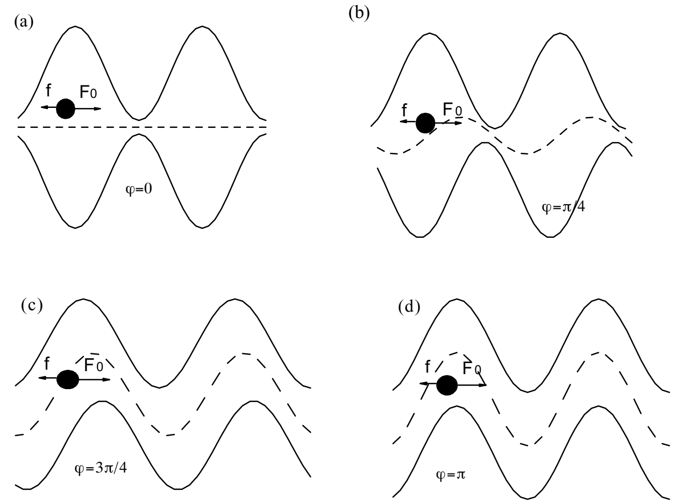

Figure 2. The schematic diagram of the channel with periodicity 2π for different values of φ. (a) $\varphi = 0$. (b) $\varphi = \pi/4$. (c) $\varphi = 3\pi/4$. (d) $\varphi = \pi$. The solid lines represent the top and bottom walls, the dashed line represents the midline of the channel.

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x)\frac{\partial P(x,t)}{\partial x} + \frac{D(x)}{k_B T}\frac{\partial A(x,t)}{\partial x}P(x,t)\right] = -\frac{\partial j(x,t)}{\partial x}. \tag{6}$$

Here $D(x)$ is x-dependent effective diffusion coefficient and when $\omega'(x) < 1$, it reads

$$D(x) = \frac{D_0}{1 + y_0'(x)^2 + (1/12)h'(x)^2}, \tag{7}$$

$D_0 = k_B T/\gamma$, the prime stands for the derivative with respect to the space variable x. The width $h(x)$ and centerline $y_0(x)$ of the tube are respectively determined by

$$h(x) = \omega_+(x) - \omega_-(x) \tag{9}$$

and

$$y_0(x) = [\omega_+(x) + \omega_-(x)]/2. \tag{10}$$

In Eq. (6), $A(x,t) = E - TS = fx - F(t)x - k_B T \ln h(x)$ is the free energy, and $E = fx - F(t)x$ is the energy, $S = k_B T \ln h(x)$ is the entropy and $h(x)$ is the dimensionless width of the tube. $j(x,t)$ is the probability current density and $P(x,t)$ is the probability density of the particle at position x and at time t, and satisfies the normalization condition and the periodicity condition $\int_0^L P(x,t)dx = 1$, $P(x,t) = P(x+L,t)$, respectively.

If $F(t)$ changes very slowly with respect to t, which means that its period is longer than any other time scale of the system. There exists a quasi-steady state. In this case, the particle current can be obtained by the method in Ref. [9].

$$j(F(t)) = \frac{k_B T\left\{1 - \exp\left[-\frac{(F(t)-f)L}{k_B T}\right]\right\}}{\left\{\int_0^L \exp\left[-\frac{(F(t)-f)x}{k_B T}\right]dx \int_x^{x+L} D^{-1}(y)\exp\left[-\frac{(F(t)-f)y}{k_B T}\right]dy\right\}}. \tag{11}$$

When $F(t) - f = 0$, from Eq. (11), we can find that $j = 0$. When $a = 0$, the channel is straight and the entropic barriers disappear, from Eq. (11), we can obtain:

$$j(F(t)) = \frac{2(F(t)-f)^2}{1 - \exp^{-2(F(t)-f)L/k_B T}}. \tag{12}$$