Current in a three-dimensional periodic tube with unbiased forces

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Transport of a Brownian particle moving along the axis of a three-dimensional asymmetric periodic tube is investigated in the presence of asymmetric unbiased forces. The reduction of the coordinates may involve not only the appearance of entropic barrier but also the effective diffusion coefficient. It is found that in the presence of entropic barrier, the asymmetry of the tube shape and the asymmetry of the unbiased forces are the two ways of inducing a net current. The current is a peaked function of temperature which indicates that the thermal noise may facilitate the transport even in the presence of entropic barrier. An optimized radius exists at the bottleneck at which the current takes its maximum value. Competition between the two opposite driving factors may induce current reversal.

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I. INTRODUCTION

Transport phenomena play a crucial role in many processes from physical and biological to social systems. There has been an increasing interest in transport properties of nonlinear systems which can extract usable work from unbiased nonequilibrium fluctuations [1–5]. In these systems, directed Brownian motion of particles is generated by nonequilibrium noise in the absence of any net macroscopic forces and potential gradients [4]. In all these studies, the potential is taken to be asymmetric in space. It has also been shown that a unidirectional current can also appear for spatially symmetric potentials if there exits an external random force either asymmetric [2] or spatially dependent [3].

Most studies have referred to the consideration of the energy barrier. The nature of the barrier depends on which thermodynamic potential varies when passing from one well to the other, and their presence plays an important role in the dynamics of the solid-state physics system. However, in some cases, such as soft condensed-matter and biological systems, the entropy barriers should be considered. The entropy barriers may appear when coarsening the description of a complex system for simplifying its dynamics. Reguera and co-workers [6] use the mesoscopic nonequilibrium thermodynamics theory to derive the general kinetic equation of a system and analyze in detail the case of diffusion in a domain of irregular geometry in which the presence of the boundaries induces an entropy barrier when approaching the dynamics by a coarsening of the description. In their recent work [7], they studied the current and diffusion of a Brownian particle in a symmetric channel with a biased external force. They found that the temperature dictates the strength of the entorpic potential, and thus an increasing of temperature leads to a reduction of the current. The previous works on entropic barriers is limited to biased external force. However, in some cases, the net current occurs in the absence of any net macroscopic forces or in the presence of unbiased forces. For example, molecular motors move along the microtubule without any net macroscopic force. The present work is extended to the study of entropic barriers to the case of unbiased forces that indicates zero force at macroscopic scale. Our emphasis is on finding conditions of obtaining a net current in the presence of entropic barriers. The asymmetry of the tube shape and the asymmetry of the unbiased fluctuations are the two driving factors for obtaining a net current. When the two driving factors compete with each other, the current may reverse its direction.

II. CURRENT IN A THREE-DIMENSIONAL PERIODIC TUBE

We consider a Brownian particle moving in a asymmetric periodic tube (Fig. 1) in the presence of an asymmetric unbiased fluctuations. Its overdamped dynamics is described by [7]

$$\eta\frac{d\vec{r}}{dt}=\vec{F}_x(t)+\sqrt{\eta k_B T}\vec{\xi}(t), \tag{1}$$

where $\vec{r}$ is the three-dimensional (3D) coordinate, η is the friction coefficient of the particle, k_B is the Boltzmann constant, T is the temperature, and $\vec{\xi}(t)$ is the Gaussian white noise with zero mean and correlation function: $\langle\xi_i(t)\xi_j(t')\rangle=2\delta_{i,j}\delta(t-t')$ for $i,j=x,y,z$. $\langle\cdots\rangle$ denotes an ensemble average over the distribution of $\vec{\xi}(t)$. $\delta(t)$ is the Dirac delta func-

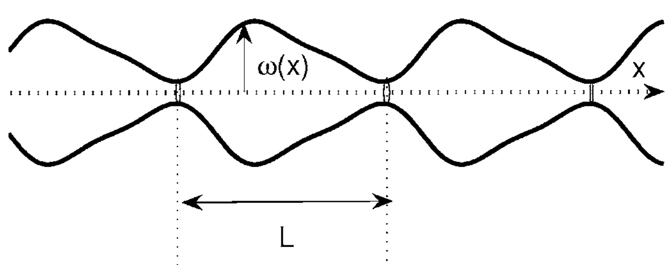

FIG. 1. Schematic diagram of a tube with periodicity L. The shape is described by the radius of the tube $\omega(x)=a[\sin(\frac{2\pi x}{L})+\frac{\Delta}{4}\sin(\frac{4\pi x}{L})]+b$. Δ is the asymmetric parameter of the tube shape.

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tion. The reflecting boundary conditions ensure the confinement of the dynamics with the tube. $\vec{F}_x(t)$ is an asymmetric unbiased external force along the x direction. $F(t)=|\vec{F}_x(t)|$ is its scalar quantity and satisfies [8,9]

$$F(t+\tau)=F(t), \qquad \int_0^\tau F(t)dt=0, \tag{2}$$

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

where τ is the period of the unbiased force, F_0 is its magnitude, and ε the temporal asymmetric parameter with $-1 \leqslant \varepsilon \leqslant 1$.

The shape of the tube is described by its radius,

$$\omega(x)=a\left[\sin\left(\frac{2\pi x}{L}\right)+\frac{\Delta}{4}\sin\left(\frac{4\pi x}{L}\right)\right]+b, \tag{4}$$

where a is the parameter that controls the slope of the tube, Δ is the asymmetry parameter of the tube shape. The radius at the bottleneck is $r_b=b-a\sqrt{1+\frac{\Delta^2}{16}}$.

The movement equation of a Brownian particle moving along the axis of the 3D tube can be described by the Fick-Jacobs equation [6,7,10,11] which is derived from the 3D (or 2D) Smoluchowski equation after elimination of y and z coordinates by assuming equilibrium in the orthogonal directions. The reduction of the coordinates may involve not only the appearance of entropic barrier, but also the effective diffusion coefficient. When $|\omega'(x)| \ll 1$, the effective diffusion coefficient reads [7,10]

$$D(x)=\frac{D_0}{[1+\omega'(x)^2]^\alpha}, \tag{5}$$

where $D_0=k_BT/\eta$ and $\alpha=1/3$ and $1/2$ for two and three dimensions, respectively.

Consider the effective diffusion coefficient and the entropic barrier, the dynamics of a Brownian particle moving along the axis of the 3D tube can be described by [6,7]

$$\frac{\partial P(x,t)}{\partial t}=\frac{\partial}{\partial x}\left(D(x)\frac{\partial P(x,t)}{\partial x}+\frac{D(x)}{k_BT}\frac{\partial A(x,t)}{\partial x}P(x,t)\right) = -\frac{\partial j(x,t)}{\partial x}, \tag{6}$$

where we define a free energy $A(x,t):=E-TS=-F(t)x-Tk_B\ln h(x)$: here $E=-F(t)x$ is the energy, $S=k_B\ln h(x)$ is the entropy, $h(x)$ is the dimensionless width $2\omega(x)/L$ in two dimensions, and the dimensionless transverse cross section $\pi[\omega(x)/L]^2$ of the tube in three dimensions. $j(x,t)$ is the probability current density. $P(x,t)$ is the probability density for the particle at position x and at time t. It satisfies the normalization condition $\int_0^L P(x,t)dx=1$ and the periodicity condition $P(x,t)=P(x+L,t)$.

If $F(t)$ changes very slowly with respect to t, namely, its period is longer than any other time scale of the system, there exists a quasisteady state. In this case, by following the method in [1–7,12], we can obtain the current

$$j(F(t))=\frac{k_BT\left[1-\exp\left(-\frac{F(t)L}{k_BT}\right)\right]}{\int_0^L h(x)\exp\left(\frac{F(t)x}{k_BT}\right)dx\int_x^{x+L}[1+\omega'(y)^2]^\alpha h^{-1}(y)\exp\left(-\frac{F(t)y}{k_BT}\right)dy}. \tag{7}$$

The average current is

$$J=\frac{1}{\tau}\int_0^\tau j(F(t))dt=\frac{1}{2}(j_1+j_2), \tag{8}$$

with

$$j_1=(1-\varepsilon)j\left(\frac{1+\varepsilon}{1-\varepsilon}F_0\right), \quad j_2=(1+\varepsilon)j(-F_0). \tag{9}$$

III. RESULTS AND DISCUSSIONS

Because the results from two and three dimensions are very similar, for the convenience of physical discussion, we now mainly investigated the current in three dimensions with $k_B=1$ and $\eta=1$.

The current J as a function of temperature T for the case $\varepsilon=0.0$ is presented in Fig. 2 for different values of asymmetric parameter of the tube shape. The curve is observed to be bell shaped, which shows the feature of resonance. When $T\to 0$, the particle cannot reach the 3D area and the effect of entropic barrier disappears and there is no current. When $T\to\infty$, the effect of the unbiased forces disappears and the current goes to zero, also. There is an optimized value of T at which the current J takes its maximum value, which indicates that the thermal noise may facilitate the particle transport even in the presence of entropic barrier. The current is negative for $\Delta<0$, zero at $\Delta=0$, and positive for $\Delta>0$. Therefore the asymmetry of the tube shape is a way of inducing a net current.

Figure 3 shows the current J as a function of the radius at the bottleneck r_b for the case $\varepsilon=0.0$ and $\Delta=1.0$. If the bottle-

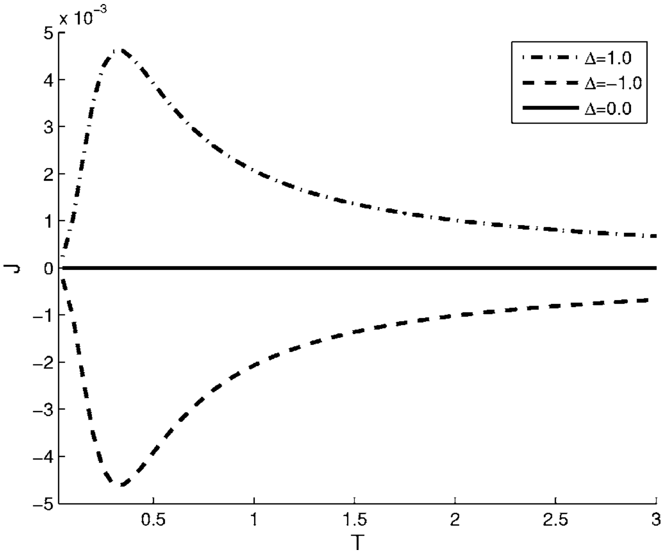

FIG. 2. Current J vs temperature T for different asymmetric parameters Δ of the tube shape at $a=1/2\pi$, $b=1.5/2\pi$, $L=2\pi$, $\alpha=1/2$, $F_0=0.5$, and $\varepsilon=0.0$.

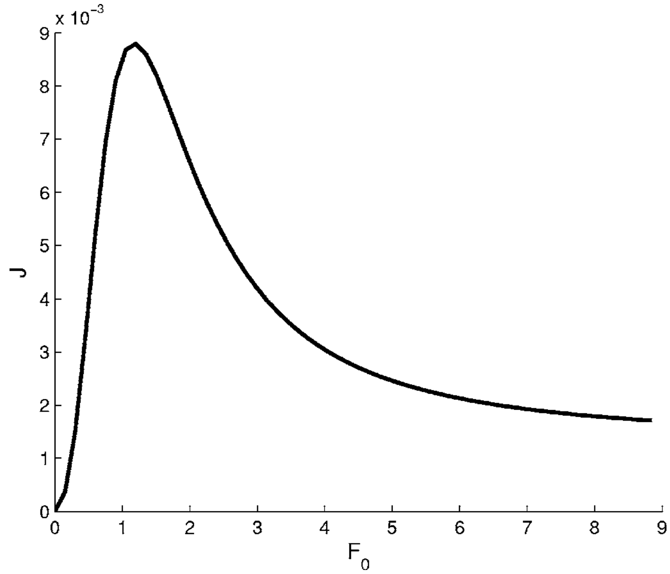

FIG. 4. Current J vs amplitude F_0 of the external force at $a=1/2\pi$, $b=1.5/2\pi$, $L=2\pi$, $\alpha=1/2$, $T_0=0.5$, and $\varepsilon=0.0$.

neck has zero the particle cannot pass through the bottleneck, so the current should be zero. When the bottleneck has infinite radius, the effect of tube shape disappears and the current tends to zero, also. Therefore the current J is a peaked function of the radius r_b at the bottleneck.

Figure 4 shows the current J vs the amplitude F_0 of the unbiased forces of for the case $\varepsilon=0.0$ and $\Delta=1.0$. When $F_0 \rightarrow 0$, only the effect of the entropic barrier exists, so the current tends to zero. The current J saturates to a certain value in the large amplitude F_0 limit. There exists an optimized value of F_0 at which the current T takes its maximum value.

The current J as a function of temperature T for the case $\Delta=0.0$ is presented in Fig. 5 for different values of asymmetric parameter ε of unbiased forces. The curve is a bell shaped function of temperature which is the same as that in Fig. 2. The asymmetry of the unbiased forces can induce a net current even when the shape of the tube is symmetric. For the asymmetry of the tube shape, the asymmetry of the external force is another way of obtaining a net current. Similarly, J is negative for $\varepsilon<0$, zero at $\varepsilon=0$, and positive for $\varepsilon>0$.

In Fig. 6, we plot the current J as a function of temperature T for different combinations of Δ and ε. When the asymmetric parameter Δ of the tube shape is positive, the current may reverse its direction on increasing temperature for negative ε. It is obvious that the current reversal may occur when a positive driving factor competes with a negative one. Therefore there may exist current reversal for $\Delta\varepsilon<0$ ($\Delta=1.0$, $\varepsilon=-0.1$; $\Delta=1.0$, $\varepsilon=-0.15$; $\Delta=1.0$, $\varepsilon=-0.2$).

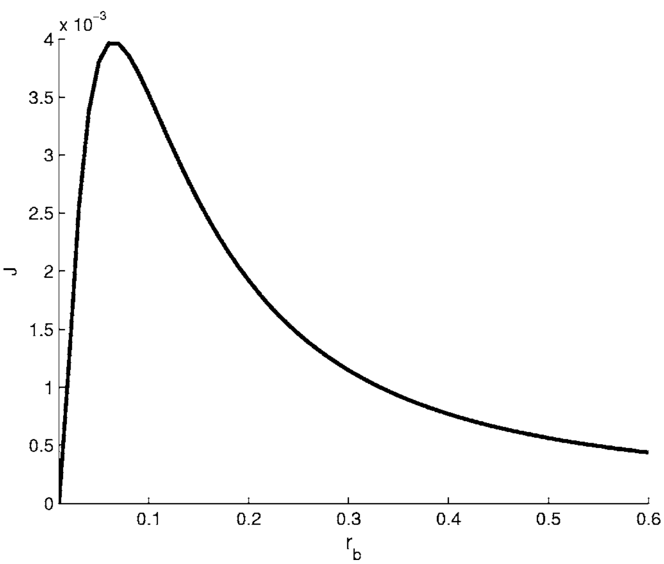

FIG. 3. Current J vs the radius r_b at the bottleneck at $a=1/2\pi$, $\alpha=1/2$, $L=2\pi$, $F_0=0.5$, $T=0.5$, $\Delta=1.0$, and $\varepsilon=0.0$.

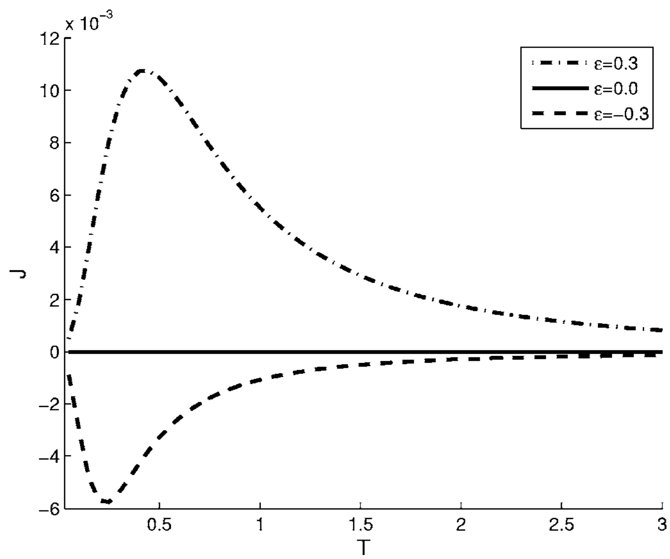

FIG. 5. Current J vs temperature T for different asymmetric parameters ε of the external force at $a=1/2\pi$, $b=1.5/2\pi$, $L=2\pi$, $\alpha=1/2$, $F_0=0.5$, and $\Delta=0.0$.

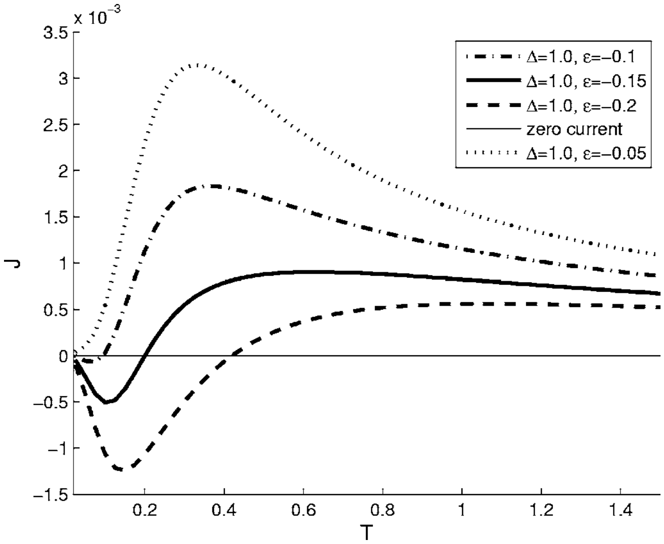

FIG. 6. Current J vs temperature T for different combinations of ε and Δ at $a=1/2\pi$, $b=1.5/2\pi$, $L=2\pi$, $\alpha=1/2$, and $F_0=0.5$.

However, $\Delta\varepsilon<0$ is not a sufficient condition for current reversal. For example, the current is always positive for $\Delta=1.0$, $\varepsilon=-0.05$.

IV. CONCLUDING REMARKS

In this paper, we study the transport of a Brownian particle moving in a 3D periodic tube in the presence of the unbiased forces. The presence of the boundaries induces an entropic barrier when approaching the exact dynamics by coarsening of the description. Both the asymmetry of the tube shape and the asymmetry of the unbiased forces are the two driving factors for obtaining a net current. When the two driving factors compete with each other, the current may reverse its direction upon increasing temperature. When the bottleneck has zero radius and infinite radius then the current tends to zero. An optimized bottleneck radius leads to a maximum current. There exists an optimize value of temperature at which the current takes its maximum value, which indicates that the thermal noise may facilitate the current. The results we have presented have a wide application in many processes [6], such as molecular motor movement through the microtubule in the absence of any net macroscopic forces [13], ion transport through ion channels [14], motion of polymers subjected to rigid constraints [15], drug release [16], and polymer crystallization [17]. In these systems, a directed transport with entropic barriers can be obtained in the absence of any net macroscopic forces or in the presence of the unbiased forces.

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