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J. Phys. A: Math. Theor. **43** (2010) 155001 (9pp) doi:10.1088/1751-8113/43/15/155001

Particle pumping driven by asymmetric unbiased external forces in a finite tube

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Received 2 November 2009, in final form 18 February 2010
Published 22 March 2010
Online at stacks.iop.org/JPhysA/43/155001

Abstract

The transport of Brownian particles in a finite tube is investigated in the presence of asymmetric unbiased external forces. The system is embedded in a finite region and bounded by two particle reservoirs. It is found that the transport phenomena under asymmetric unbiased external forces exhibit peculiar behaviours. In a spatially symmetric tube, the particles can be pumped by asymmetric unbiased forces. Both spatial asymmetry of a tube and temporal asymmetry of unbiased external forces are the two driving factors for pumping particles from a reservoir at low concentration to one at the same or higher concentration. The interplay between these two factors can induce peculiar phenomena.

PACS numbers: 05.60.Cd, 02.50.Ey, 05.40.Jc

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Noisy transport in ratchet systems, which are far from equilibrium, has been an active field of research over the last decade [1–3]. In these spatially finite structures, the directed motion of particles can be induced by zero-mean nonequilibrium fluctuations and noise.

The idea of applying the ratchet mechanism to model pumps has already appeared in the literature [4–10]. Prost and co-workers researched the transport of an asymmetric pump with a simple two-level model and quantified how vectorial symmetry plus dissipation creates a macroscopic motion [4]. Kosztin and Schulten [5] investigated the fluctuation-driven molecular transport through an asymmetric potential pump and three transport mechanisms: driven by a potential gradient, by an external periodic force and by nonequilibrium fluctuations. Astumian and Derenyi [6] studied a chemically driven molecular electron pump in which charge can be pumped through a tiny gated portal from a reservoir at low electrochemical potential to one at the same or higher electrochemical potential by cyclically modulating the portal and gate energies. Rey and co-workers [7] investigated the nonadiabatic electron heat pump. Wambaugh and co-workers [8] studied the transport of fluxons in superconductors by alternating current rectification. Kjelstrup and co-workers [9] studied the active transport in slipping biological pumps and shown that how heating as well as cooling effects can be associated with the pump operation. Sancho and Gomez-Marin [10] researched a model for a Brownian pump powered by a flashing ratchet mechanism. Brownian particles moving in an asymmetric finite tube in the presence of an unbiased external force were investigated by Ai and co-workers [11].

The previous works on pump were focused on the symmetric unbiased force. In the present work, we extend the previous work on the Brownian pump to the case of asymmetric unbiased forces. We emphasize on finding how the interplay between spatial asymmetry and temporal asymmetry affects the current and the pumping capacity of the system.

2. General analysis

We consider overdamped Brownian particles moving in a finite tube in the presence of asymmetric unbiased external forces (figure 1). The tube is embedded in a finite region and bounded by two particle reservoirs. In general, the overdamped dynamics is well governed by the following Langevin equations expressed in a dimensionless form [2, 12]:

$$\eta \frac{\mathrm{d}x}{\mathrm{d}t} = F(t) + \sqrt{\eta K_B T}\xi_x(t), \tag{1}$$

$$\eta \frac{\mathrm{d}y}{\mathrm{d}t} = \sqrt{\eta K_B T}\xi_y(t), \tag{2}$$

$$\eta \frac{\mathrm{d}z}{\mathrm{d}t} = \sqrt{\eta K_B T}\xi_z(t), \tag{3}$$

where x, y, z are the three-dimensional (3D) coordinates, t is the time, K_B is the Boltzmann constant, T is the absolute temperature, η is the viscous friction coefficient (static mobility) and $\xi_{x,y,z}(t)$ is the Gaussian white noise with zero mean and a correlation function $\langle \xi_i(t)\xi_j(t')\rangle = 2\delta_{ij}\delta(t-t')$ for $i, j = x, y, z$ $\langle\cdots\rangle$ denotes an ensemble average over the distribution of noise. $\delta(t)$ is the Dirac delta function. The reflecting boundary conditions ensure the confinement of the dynamics within the tube. $F(t)$ is a temporally asymmetric unbiased external force along the x direction which may be imparted as a result of energy gained via ATP hydrolysis in biological pumps and satisfies

$$F(t) = \begin{cases} \dfrac{1+\varepsilon}{1-\varepsilon}F_0, & n\tau \leqslant t < n\tau + \dfrac{1}{2}\tau(1-\varepsilon), \\ -F_0, & n\tau + \dfrac{1}{2}\tau(1-\varepsilon) < t \leqslant (n+1)\tau, \end{cases} \tag{4}$$

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

The shape of the tube is described by its radius

$$\omega(x) = a\sin\left(\frac{2\pi x}{L}\right) + b, \qquad x_0 \leqslant x \leqslant x_0 + L, \tag{5}$$

where a is the parameter controlling the slope of the tube, b is the parameter that determines the half width at the bottleneck. L is the length of the tube and x_0 is the coordinate of the left end which describes the asymmetry of the tube.

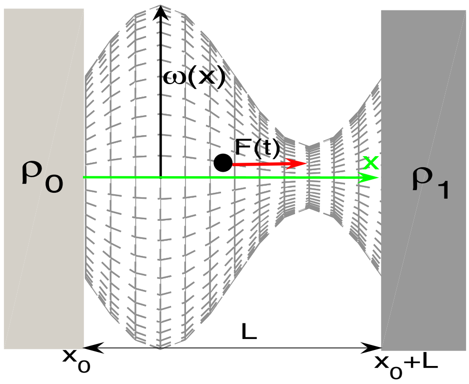

Figure 1. Scheme of the pumping device: a spatially asymmetric tube is embedded in a finite region of length L and bounded by two particle reservoirs of concentrations ρ_0 and ρ_1. The shape of the tube is determined by its radius $\omega(x)$ and the left-end coordinate x_0 of the tube. The particles in the tube are powered by temporally asymmetric unbiased external forces $F(t)$.

The movement equation of a Brownian particle moving along the axis of the 3D tube can be described by the Fick–Jacobs equation [11–14] which is derived from the 3D (or 2D) Smoluchowski equation after the 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 an entropic barrier, but also the effective diffusion coefficient. When $|\omega'(x)| \ll 1$, the effective diffusion coefficient reads [12–15]

$$D(x) = \frac{D_0}{[1+\omega'(x)^2]^\alpha}, \tag{6}$$

where $D_0 = k_B T/\eta$ and $\alpha = 1/3, 1/2$ for 2D and 3D, respectively.

Considering 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 [11–13]

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x)\frac{\partial \rho(x,t)}{\partial x} + \frac{D(x)}{k_B T}\frac{\partial A(x,t)}{\partial x}\rho(x,t)\right] = -\frac{\partial j(x,t)}{\partial x}, \tag{7}$$

where we define a free energy $A(x,t) := E - TS = -F(t)x - Tk_B \ln h(x)$ [12–14]. Here, $E = -F(t)x$ is the energy, $S = k_B \ln h(x)$ is the entropy and $h(x)$ is the dimensionless transverse cross section $\pi[\omega(x)/L]^2$ of the tube in three dimensions. $j(x,t)$ is the probability current and $\rho(x,t)$ is the particle concentration.

If its period is longer than any other time scale of the system, namely $F(t)$ changes very slowly with respect to t, there exists a quasi-steady state. In the steady state, the concentration is just a function of the space thus, and the flux becomes a constant j. The concentration $\rho(x)$ follows a first-order nonhomogeneous linear differential equation whose formal solution is [10]

$$\rho(x) = \exp\left[-\int_{x_0}^{x}\frac{A'(z)}{k_B T}\,\mathrm{d}z\right] \times \left\{C_0 - j\int_{x_0}^{x}\frac{\mathrm{d}z}{D(z)}\exp\left[\int_{x_0}^{x}\frac{A'(y)}{k_B T}\,\mathrm{d}y\right]\right\}. \tag{8}$$

The unknown constant c_0 can be found by imposing the left reservoir concentration $\rho_0 = \rho(x_0)$ and the right concentration $\rho_1 = \rho(x_0 + L)$ as fixed boundary conditions [9], although different from the typical Brownian motors, the boundary conditions are not periodic nor the normalized conditions are imposed. Then, $c_0 = \rho(x_0)$ and

$$j(F_0) = \frac{k_B T\left[\rho_0 - \rho_1 \,\mathrm{e}^{\frac{F_0 L}{k_B T}}\right]}{\int_{x_0}^{x_0+L} [1+\omega'(x)^2]^{\alpha}\,\mathrm{e}^{-\frac{F_0(x-x_0)}{k_B T}}\left[\frac{\omega(x_0)}{\omega(x)}\right]^2 \mathrm{d}x}. \tag{9}$$

The average current is

$$J = \frac{1}{\tau}\int_0^{\tau} j(F(t))\,\mathrm{d}t = \frac{1}{2}(j_1 + j_2), \tag{10}$$

where

$$j_1 = (1-\varepsilon)\, j\left(\frac{1+\varepsilon}{1-\varepsilon}F_0\right), \qquad j_2 = (1+\varepsilon)\, j(-F_0). \tag{11}$$

We consider the situation in which J is equal to zero in studying the pumping capacity, which corresponds to the case in which the pump maintains the maximum concentration difference between the two reservoirs across the channel with no net leaking of a particle. The method is the same as that in [10] and [11]. This situation is analogous to the stalling force in Brownian motors.

From equations (8)–(10), we can obtain

$$\frac{\rho_1}{\rho_0} = \frac{\int_{x_0}^{x_0+L}[1+\omega'(x)^2]^{\alpha}\left[\mathrm{e}^{-\frac{1+\varepsilon}{1-\varepsilon}\frac{F_0(x-x_0)}{k_B T}} + \mathrm{e}^{\frac{F_0(x-x_0)}{k_B T}}\right]\left[\frac{\omega(x_0)}{\omega(x)}\right]^2 \mathrm{d}x}{\mathrm{e}^{\frac{F_0 L}{k_B T}}\int_{x_0}^{x_0+L}[1+\omega'(x)^2]^{\alpha}\,\mathrm{e}^{-\frac{1+\varepsilon}{1-\varepsilon}\frac{F_0(x-x_0)}{k_B T}}\left[\frac{\omega(x_0)}{\omega(x)}\right]^2 \mathrm{d}x + \mathrm{e}^{-\frac{1+\varepsilon}{1-\varepsilon}\frac{F_0 L}{k_B T}}\int_{x_0}^{x_0+L}[1+\omega'(x)^2]^{\alpha}\,\mathrm{e}^{\frac{F_0(x-x_0)}{k_B T}}\left[\frac{\omega(x_0)}{\omega(x)}\right]^2 \mathrm{d}x}. \tag{12}$$

3. Results and discussions

Since the results from 2D are similar to 3D, we mainly focused on the 3D case. For simplicity, we take $k_B = 1$, $\eta = 1$ and $L = 2\pi$ throughout the study.

The current J acts as a function of the asymmetric parameter ε of the external forces in figure 2(*a*) for the spatially symmetric tube at $\rho_0 = \rho_1$. The current is negative for $\varepsilon < 0$, while the current is positive for $\varepsilon > 0$. It shows that the current can be reversed by the asymmetric unbiased forces, even if the tube is spatially symmetric. The two curves ($x_0 = \pi/2$, $x_0 = 3\pi/2$) intersect each other at two positions: one is at $J = 0$, $\varepsilon = 0$, and the other is at $J = 0.098\,91$, $\varepsilon = 0.18$. Figure 2(*b*) shows the concentration ratio ρ_1/ρ_0 as a function of the asymmetric parameter ε of the external unbiased forces for a spatially symmetric tube at $J = 0$. We can find that the concentration ratio ρ_1/ρ_0 increases monotonically with the increase of the asymmetric parameter ε. The ratio of the concentrations ρ_1/ρ_0 is greater than 1 for $\varepsilon < 0$, and less than 1 for $\varepsilon > 0$. Namely, even the tube is spatially symmetric, its pumping capacity can be induced by the asymmetric unbiased forces. Both curves for $x_0 = \pi/2$ and $x_0 = 3\pi/2$ intersect each other at $\varepsilon = 0$, $\rho_1/\rho_0 = 1$. The condition corresponding this intersection position is that both the tube and unbiased forces are symmetric. That is to say, the pumping capacity of the system disappears.

In order to describe the current transformation in detail, the current J contours on the x_0–ε plane at $\rho_1 = \rho_0$ in this system are shown in figure 3. Different values of the initial coordinate x_0 represent different tube shapes. When $x_0 = \pi/2$ or $x_0 = 3\pi/2$, the tube is symmetric in space. In the above discussion, the influence of the spatial asymmetry of a tube on the current is investigated. Figure 3 shows that both the asymmetry of the space and the temporal asymmetry of the unbiased forces are the two driving factors obtaining a net current.

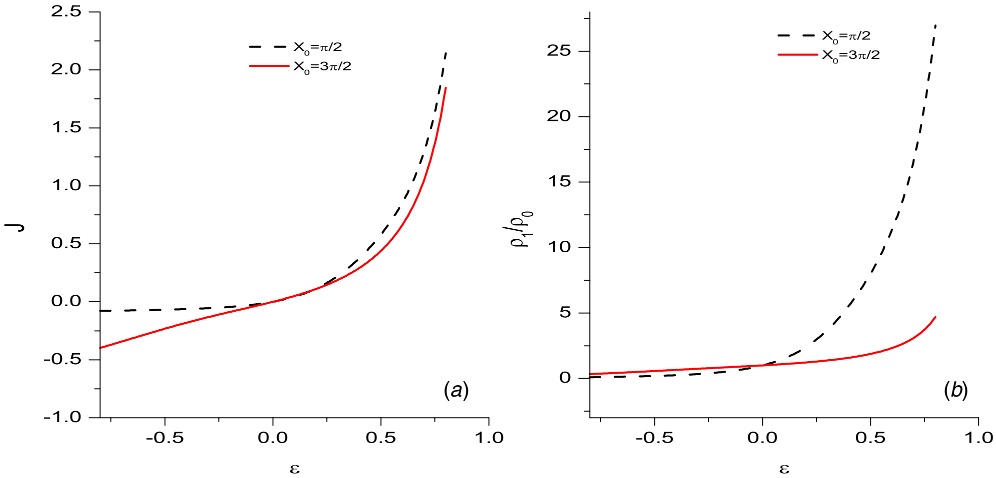

Figure 2. (*a*) Current J as a function of ε for different values of x_0 at $a = 1/2\pi$, $b = 1.5/2\pi$, $\alpha = 1/2$, $T = 0.5$, $F = 0.5$, $\rho_1 = 1$ and $\rho_0 = 1$. (*b*) The ratio of concentrations as a function of ε for different values of x_0 at $a = 1/2\pi$, $b = 1.5/2\pi$, $\alpha = 1/2$, $T = 0.5$, $F = 0.5$ and $J = 0$.

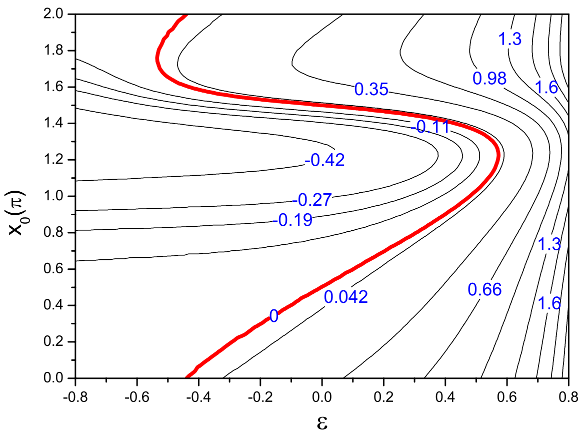

Figure 3. Current J contours on the x_0–ε plane at $a = 1/2\pi$, $b = 1.5/2\pi$, $\alpha = 1/2$, $T = 0.5$, $F = 0.5$ and $\rho_1/\rho_0 = 1$. The thick solid line indicates $J = 0$ contour.

When the two driving factors compete with each other, the current may reverse its direction. The thick solid line indicates $J = 0$ contour. The positive driving factor and the negative one cancel each other out, so the current disappears, at all points of this curves. In the region on the left of the curve corresponding to zero current, all currents are negative. In the other region, however, the currents are positive. For a given spatially asymmetric parameter x_0, the current may undergo a reversal in direction. When $\varepsilon = 0.0$, the system comes back to a channel Brownian pump powered by symmetric unbiased external forces, and the results are the same as our previous ones [11].

Similarly, in order to illustrate the pumping capacity in detail, the concentration ratio ρ_1/ρ_0 contours are shown in figure 4, the thick solid line indicates $\rho_1/\rho_0 = 1$ contour, and this representative curve describes the competition of the two driving factors: the asymmetry

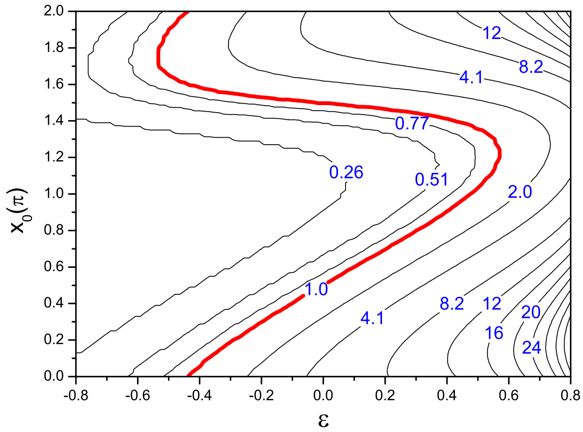

Figure 4. The concentration ratio ρ_1/ρ_0 contours on the x_0–ε plane at $a = 1/2\pi$, $b = 1.5/2\pi$, $\alpha = 1/2$, $T = 0.5$, $F = 0.5$ and $J = 0$. The thick solid line indicates $\rho_1/\rho_0 = 1$ contour.

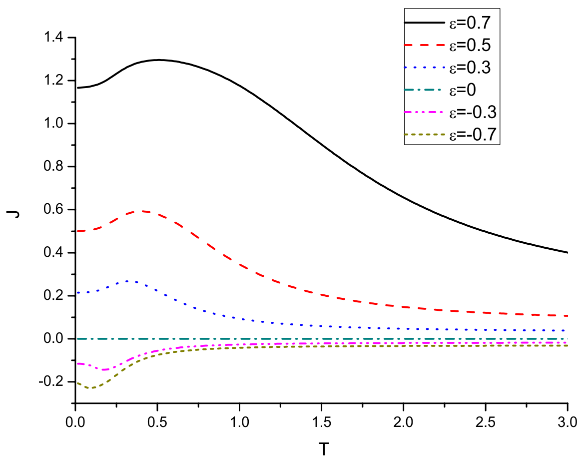

Figure 5. Current J versus temperature T for different asymmetric parameters ε of unbiased external forces at $a = 1/2\pi$, $b = 1.5/2\pi$, $\alpha = 1/2$, $F = 0.5$, $x_0 = \pi/2$, $\rho_1 = 1$ and $\rho_0 = 1$.

of the space and the asymmetry of the unbiased forces. When $\varepsilon = 0.0$, the concentration ratio ρ_1/ρ_0 is greater than 1 for $0 \leqslant x_0 < \pi/2$ and $3\pi/2 \leqslant x_0 < 2\pi$, equal to 1 at $x_0 = \pi/2$ and $3\pi/2$, and less than 1 for $\pi/2 < x_0 < 3\pi/2$. And when $x_0 = \pi/2$ or $3\pi/2$, the concentration ratio is greater than 1 for $\varepsilon > 0$, equal to 1 at $\varepsilon = 0$ and less than 1 for $\varepsilon < 0$. Thus, the pumping direction is positive ($\rho_1 > \rho_0$) for $0 \leqslant x_0 < \pi/2$ or $3\pi/2 \leqslant x_0 < 2\pi$; further, when $\varepsilon > 0$, the two driving factors will both promote the growth of ρ_1/ρ_0. Otherwise, the pumping direction is negative ($\rho_0 > \rho_1$) for $\pi/2 < x_0 < 3\pi/2$; when $\varepsilon < 0$, the two driving factors will both promote the growth of ρ_0/ρ_1. It is obvious that the pumping direction may reverse when a positive driving factor competes with a negative one; when $\rho_1/\rho_0 = 1$, the pumping capacity disappears.

In figure 5 we plot the current as a function of the temperature T at $x_0 = \pi/2$ for different values of the asymmetric parameter ε of unbiased external forces. The curves are

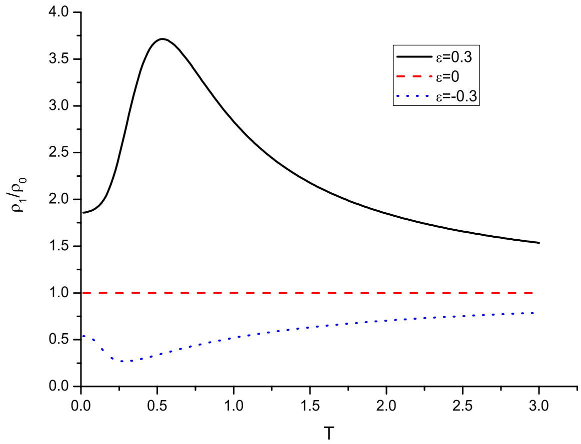

Figure 6. Ratio of concentrations as a function of T for different asymmetric parameters ε of unbiased external forces at $a = 1/2\pi$, $b = 1.5/2\pi$, $\alpha = 1/2$, $F = 0.5$, $x_0 = \pi/2$ and $J = 0$.

the bell-shaped function of temperature. The asymmetry of the unbiased forces can induce a net current, even when the tube is symmetric. Except for the asymmetry of the tube, the asymmetry of the external forces is another way of obtaining a net current (as can be seen from figure 3). When $T \longrightarrow 0$, even if $T = 0$, the particles can move from one particle reservoir to the other. Another significant feature shown in the figure is that the current is negative for $\varepsilon < 0$, and positive for $\varepsilon > 0$, which indicates that the asymmetry of the external forces may affect the direction of the current. When $\varepsilon = 0$, the unbiased forces and the shape of the tube are symmetric, and the system is still at equilibrium, which makes the current zero, even though the temperature is high. When $T \longrightarrow \infty$, the intensity of noise is so strong that the contribution of the asymmetric unbiased external force to the current can be neglected. In other words, the noise is dominant in the system, which takes the nonequilibrium system to equilibrium again, resulting in zero current. Therefore, there is an optimized value of T at which the current takes its maximum value, which indicates that the thermal noise can facilitate the current.

Figure 6 shows the ratio of concentrations as a function of T for different asymmetric parameters ε of unbiased external forces at $J = 0$, $x_0 = \pi/2$. The curves are the bell-shaped function of the temperature too. Even when the tube is symmetric, the asymmetry of the unbiased forces ($\varepsilon = 0.3$, $\varepsilon = -0.3$) can induce $\rho_1/\rho_0 \neq 0$. For all temperatures, ρ_1/ρ_0 is less than 1 for $\varepsilon < 0$, equal to 1 at $\varepsilon = 0$ and greater than 1 for $\varepsilon > 0$. When $T \longrightarrow 0$, even if $T = 0$, the system still possesses a pumping capacity, except for $\varepsilon = 0$. The particle transports from the left particle reservoir to the right for $\varepsilon = 0.3$, while it transports from the right particle reservoir to the left for $\varepsilon = -0.3$. When $T \longrightarrow \infty$, the effect of the asymmetric unbiased external force disappears and the pumping capacity becomes zero. Therefore, there is an optimized value of T at which the ratio takes its maximum value, which indicates that the thermal noise with proper intensity can facilitate the particle transport.

4. Concluding remarks

In this paper, we demonstrated that transport phenomena in a finite tube under asymmetric unbiased external forces exhibit some features that are radically different from conventional transport. The pumping device is embedded in a finite region and bounded by two particle reservoirs. It is found that, in the spatially symmetric tube, the particles transporting from one concentration reservoir to the other can be induced by the asymmetry of unbiased forces ($\varepsilon \neq 0$). We can find that the sign of the current is determined by the driving factor in the dominant position between the spatial asymmetry and the temporal asymmetry. When the two driving factors compete with each other, the current may reverse its direction. With regard to the pumping capacity, both the spatial asymmetry and the temporal asymmetry of unbiased forces are the two driving factors affecting the ratio of the concentrations. It is obvious that the pumping direction may reverse when a positive driving factor competes with a negative one; when $\rho_1/\rho_0 = 1$, the pumping capacity disappears. It will create a current and pumping capacity as long as the equilibrium of the system we presented is destroyed by spatial asymmetry and/or temporal asymmetry. We can find that there are some different optimized values of temperature T for different values of ε which give the maximum ratio of ρ_1/ρ_0 or the maximum current. This is due to the competition between the two factors.

The model is too simple to provide a realistic description of real systems. However, the predicted effects in our model may be observed in many processes, such as the vortex ratchet in a superconductor [16], gating ratchet with cold atoms in optical lattice [17], diffusion of ions and macromolecular solutes through the channels in biological membranes [18], transport in zeolites [19] and diffusion in man-made periodic porous materials [20].

Acknowledgments

The work was supported by the National Natural Science Foundation of China under grant no 30600122 and GuangDong Provincial Natural Science Foundation under grant no 06025073.

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