Current control in a two-dimensional channel with nonstraight midline and varying width

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Current controlling in a two-dimensional channel with non-straight midline and varying width

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Abstract

Transport of overdamped Brownian particles in a two-dimensional channel with non-straight midline and narrow varying width is investigated in the presence of an asymmetric unbiased external force. In the adiabatic limit, we obtain the analytical expression of the directed current. It is found that the current is manipulated by changing the phase shift between the top and bottom walls of the channel. As the phase shift is increased from 0 to π, the variation of the channel width decreases and the current also decreases. Remarkably, the current is always zero when the phase shift is equal to π, where the entropic barrier disappears. In addition, the temporal asymmetric parameter of the unbiased force not only determines the direction of the current but also affects its amplitude.

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I. INTRODUCTION

Particle transport in narrow corrugated channels has attracted increasing attention in recent years due to its important in many processes from biology and chemistry to nanotechnology [1]. Generally speaking, the corrugated channels fall into two categories depending on the geometry of the channel wall: Smoothly corrugated channels [2–21] and compartmentalized channels [22–29]. In smoothly corrugated channels, the movement equation of Brownian particles can be described by the Fick-Jacobs equation [2–21] which is derived from the three-dimensional (3D) or two-dimensional (2D) Smoluchowski equation after elimination of y and z coordinates by assuming equilibrium in the orthogonal directions. The reduction of the coordinates can involve the appearance of entropic barrier and smoothly corrugated channels can also be called entropic channels. In contrast to the smoothly corrugated channels, the compartmentalized channels have sharp boundary profiles. The diffusion of Brownian particles in compartmentalized channels cannot be reduced to an effective one-dimensional (1D) kinetic process directed along the axis.

Most studies have considered the corrugated channels with the straight midline. However, the channels that occur in nature as a rule have a curved midline and artificially produced channels do as well, the diffusion of Brownian particles in a 2D channel with non-straight midline and varying width has attracted growing attention [30–34]. Diffusion in a 2D non-straight midline channel can also be reduced to an effective 1D equation of motion and the effective diffusivity includes a contribution that comes from variations in the channel midline height $y_0(x) = [\omega_+(x) + \omega_-(x)]/2$ as well as the well-known term stemming from changes in the channel width $h(x) = \omega_+(x) - \omega_-(x)$, where $\omega_+(x)$ and $\omega_-(x)$ are the top and bottom walls of the channel respectively [30, 31]. Using the projection method, Dagdug and Pineda [32] obtained a general expression for the effective diffusion coefficient for an asymmetric 2D channel. In their later work [33], using Brownian dynamics simulation, they evaluated the accuracy of the theoretical effective diffusion coefficient for 2D, tilted, asymmetric, varying-width channels formed by straight walls and established the domain of applicability of both the 1D description and the effective diffusion coefficient formulas. Motivated by these works, we study the current induced by an asymmetric unbiased external force in the 2D channel with the non-straight midline and varying width. We emphasize on finding how the asymmetry of the unbiased force and the phase shift between the top and bottom walls of the channel affect the directed transport.

II. MODEL AND METHODS

We consider overdamped Brownian particles moving in a 2D channel with the curved midline and narrow varying width(see Fig.2). The particles are subjected to an asymmetric unbiased external force $F(t)$ along the longitudinal x direction. Since most of the molecular transport occurs in the overdamped regime, we can safely neglect inertial effect [34]. The corresponding overdamped stochastic dynamics is described by the Langevin equations in the dimensionless form:

$$\eta\frac{dx}{dt} = F(t) + \sqrt{\eta k_B T}\xi_x(t), \tag{1}$$

$$\eta\frac{dy}{dt} = \sqrt{\eta k_B T}\xi_y(t), \tag{2}$$

where x, y are coordinates, η the friction coefficient of the particle, T the temperature, and k_B the Boltzmann constant. $\xi_{x,y}(t)$ is 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 $i, j = x, y$. $\langle\cdots\rangle$ denotes an ensemble average over the distribution of noise. The reflecting boundary conditions ensure the confinement of the dynamics within the channel.

$F(t)$ is an asymmetric unbiased external force [shown in Fig.1] along the x direction and satisfies [20, 21, 35]

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

where τ is the period, F_0 is the amplitude, and ε is the temporal asymmetric parameter within [-1,1). The unbiased force means that its mean value is equal to zero ($\langle F(t)\rangle = 0$). $F(t)$ is temporal symmetric at $\varepsilon = 0$.

The shape of the channel is determined by its wall functions $\omega_+(x)$ and $\omega_-(x)$. The top wall $\omega_+(x)$ and the bottom $\omega_-(x)$ are

$$\omega_+(x) = a(1-\cos x) + b, \tag{4}$$

and

$$\omega_-(x) = -\{a[1-\cos(x+\varphi)] + b\}, \tag{5}$$

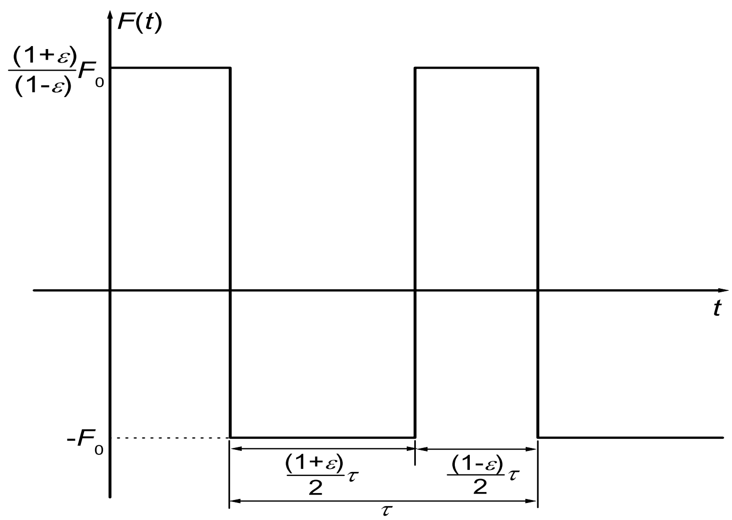

FIG. 1. Schematic diagram of the asymmetric unbiased external force. τ is the period, F_0 is the amplitude, and ε is the temporal asymmetric parameter.

where a is the parameter that controls the slope of the walls, b can control the channel width at the bottleneck, and φ is the phase shift between the top and bottom walls. The shapes of the channel are shown in Fig. 2 for different values of φ.

The dynamics of particles in confined channel can be described by the Fick-Jacobs equation which is derived from the 2D Smoluchowski equation after elimination of y coordinates by assuming equilibrium in the transverse directions. The reduction of the coordinates may involve not only the appearance of an entropic barrier but also the effective diffusion coefficient. The effective diffusion coefficient in a narrow 2D channel with non-straight midline and varying width is [30–33]

$$D(x) = \frac{D_0}{1 + y_0'(x)^2 + \frac{1}{12}h'(x)^2}, \tag{6}$$

where $D_0 = k_B T/\eta$ and the prime stands for the first derivative of x. The width $h(x)$ and centerline $y_0(x)$ of the channel are respectively determined by

$$h(x) = \omega_+(x) - \omega_-(x), \tag{7}$$

and

$$y_0(x) = [\omega_+(x) + \omega_-(x)]/2. \tag{8}$$

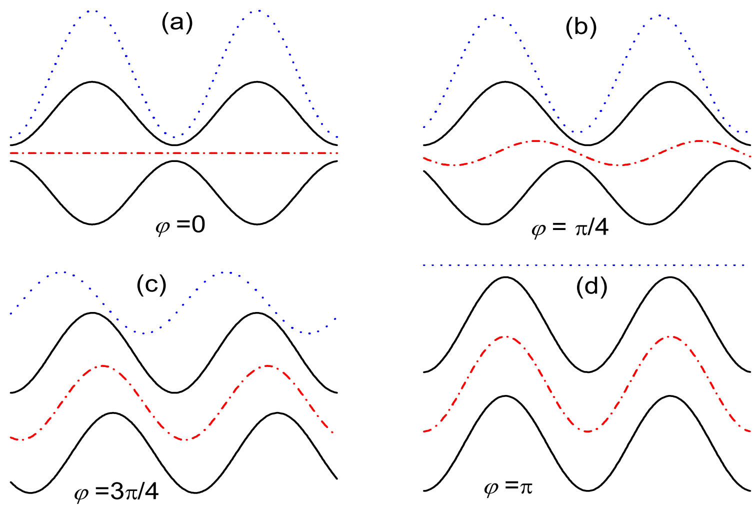

FIG. 2. (color online). Schematic diagram of the channel with periodicity 2π for different values of φ. (a) $\varphi = 0$. (b) $\varphi = \pi/4$. (c) $\varphi = 3\pi/4$. (d) $\varphi = \pi$. The solid lines (black) represent the top and bottom walls, the dashed line (blue) represents the width, and the dash-dotted line (red) the midline of the channel.

Note that if we use the Eq.(7) in reference [33], the same results are also obtained.

Considering the effective diffusion coefficient, the entropic barrier, and the asymmetric unbiased external force, the Fick-Jacobs equation can be expressed as [2–8, 20, 21]

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}[D(x)\frac{\partial P(x,t)}{\partial x} + \frac{D(x)}{k_B T}\frac{\partial A(x)}{\partial x}P(x,t)] = -\frac{\partial j(x,t)}{\partial x}, \tag{9}$$

where we define a free energy $A(x) := E - TS = -F(t)x - k_B T \ln h(x)$. Here, $E = -F(t)x$ is the energy and $S = k_B \ln h(x)$ is the entropy, where $h(x)$ is the dimensionless width of the channel. $P(x,t)$ is the probability density of the particle at position x and time t. It satisfies the normalization condition $\int_0^{2\pi} P(x,t)\mathrm{d}x = 1$ and the periodicity condition $P(x,t) = P(x + 2\pi, t)$. $j(x,t)$ is the probability current and it can be expressed as follows:

$$j(x,t) = -[D(x)\frac{\partial P(x,t)}{\partial x} + \frac{D(x)}{k_B T}\frac{\partial A(x)}{\partial x}P(x,t)]. \tag{10}$$

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, we can obtain the current [2–7, 20, 21, 36–42]

$$j(F(t)) = \frac{1-\exp(\frac{-2\pi F(t)}{k_BT})}{\int_0^{2\pi}\exp[-\frac{A(x)}{k_BT}]\mathrm{d}x\int_x^{x+2\pi}D^{-1}(y)\exp[\frac{A(y)}{k_BT}]\mathrm{d}y}. \tag{11}$$

From Eq.(3), we can obtain the average current,

$$J = \frac{1}{\tau}\int_0^{\tau} j(F(t))\mathrm{d}t = \frac{1}{2}[(1-\varepsilon)j(\frac{1+\varepsilon}{1-\varepsilon}F_0) + (1+\varepsilon)j(-F_0)], \tag{12}$$

which is the main mathematical result of this paper.

III. RESULTS AND DISCUSSIONS

We will firstly discuss the limitations of the approach they follow in terms of tube profile and drive intensity. The Fick-Jacobs equation is effective for treating diffusion in a channel when the wall shape $\omega(x)$ does not change too fast, i.e., the $|\omega'(x)|$ is small enough. The Fick-Jacobs equation fails when $|\omega'(x)|$ is larger than 1 [8]. The $\omega'(x)$ in the present work are $\frac{1}{2\pi}\sin x$ and $-\frac{1}{2\pi}\sin(x+\varphi)$. Both values of $|\omega'(x)|$ are in the interval $[0, \frac{1}{2\pi}]$, so that the reduced probability density $P(x,t)$ obeys the Fick-Jacobs equation.

Similarly, as the external force increases, the particles are not homogeneously distributed in the transverse direction and the Fick-Jacobs equation also fails [2, 13]. For our channel, the validity criterion of the external force F_c is given by [5]

$$F_c = \frac{k_BTL}{2(a+b)^2+a^2}[1-\frac{a^2}{2}]. \tag{13}$$

Submitting $k_BT = 0.5, L = 2\pi$, $a = \frac{1}{2\pi}$ and $b = \frac{0.25}{2\pi}$ into Eq. (13), the F_c is roughly equal to 30. In our paper, $F_0 = 1$, which is far less than F_c, so that the Fick-Jacobs equation holds.

Figure 3 shows the current J as a function of the temporal asymmetric parameter ε of the driving force for different values of φ. It is found that the current J is negative for $\varepsilon < 0$, zero at $\varepsilon = 0$, and positive for $\varepsilon > 0$. Especially, for $\varepsilon = -1$, J=$j(0)$=0, therefore, when $\varepsilon < 0$, there exists a value of ε at which the current J takes its extreme value (Fig.3(a)). When $\varepsilon > 0$, the current J increases monotonously with the increase of ε (Fig.3(b)). Thus we can obtain current reversals by varying the parameter ε.

Figure 4 describes the current J versus the phase shift φ for different values of a. It is found that as φ is increased, the bell shaped structure in the current amplitude is presented.

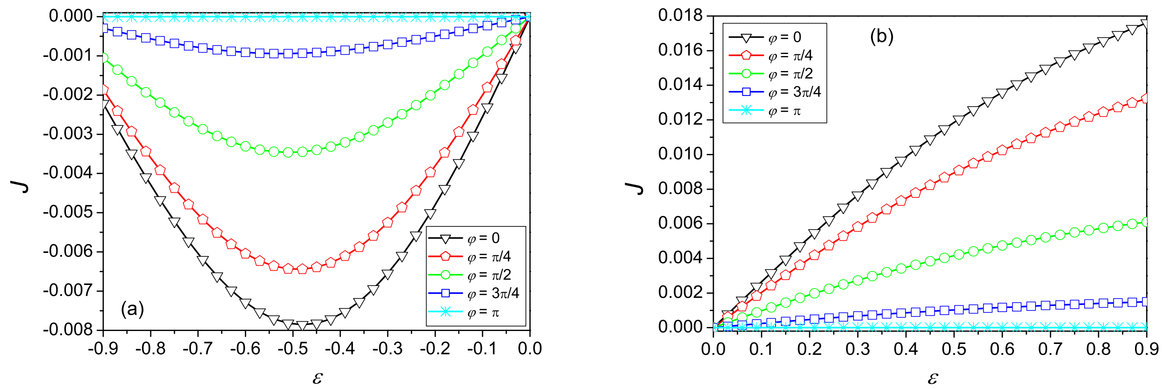

FIG. 3. (color online). Current J as a function of ε for different values of φ. (a) $-0.9 \leq \varepsilon \leq 0$. (b) $0 \leq \varepsilon \leq 0.9$. The other parameters are $a = 1/(2\pi), b = 0.25/(2\pi), k_B T = 0.5$, and $F_0 = 1$.

When $\varphi = 0$ or 2π, the current J takes its maximum value. For $\varphi = \pi$, there is no change in the width (Fig.2(d)), namely, $h'(x) = 0$, the effect of entropic barrier disappears. In addition, the external force $F(t)$ is unbiased and its mean value is equal to zero. These two factors result in the current J goes to zero at $\varphi = \pi$. The results indicate that the phase shift φ only controls the amplitude of the current.

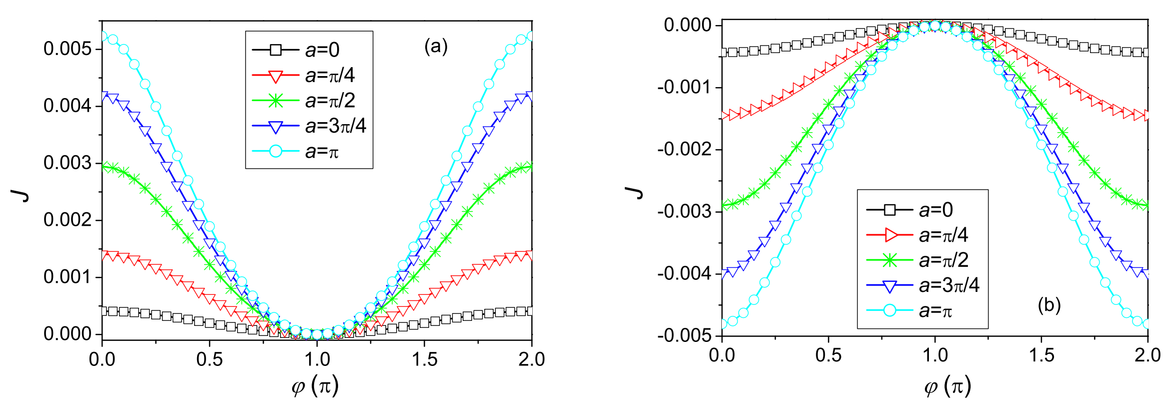

FIG. 4. (color online). Current J as a function of φ for different values a. (a) $\varepsilon = 0.2$. (b) $\varepsilon = -0.2$. The other parameters are $b = 0.25/(2\pi)$, $k_B T = 0.5$, and $F_0 = 1$.

In order to illustrate the competition between the asymmetric parameter ε and the phase shift φ, the current contours on the φ-ε plane are shown in Fig.5. It is found that the

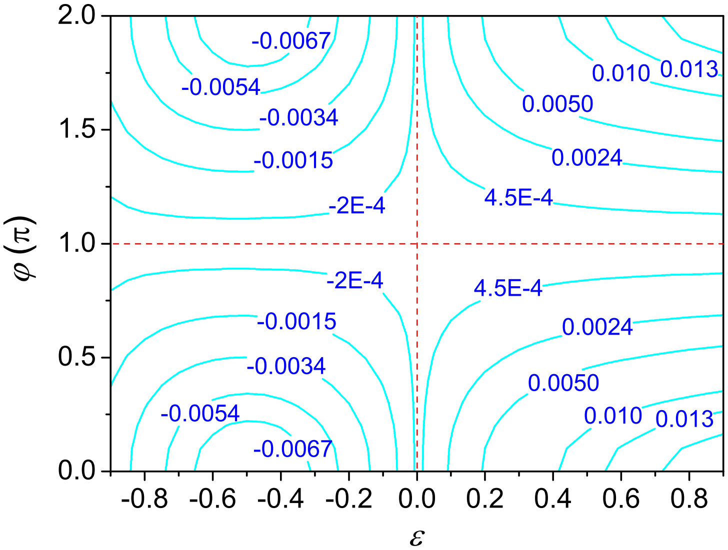

FIG. 5. (color online). Current contours on the φ-ε plane at $a = 1/2\pi, b = 0.25/2\pi, k_BT = 0.5$, and $F_0 = 1$.

current J is always positive for $\varepsilon > 0$, zero at $\varepsilon = 0$, and negative for $\varepsilon < 0$. Remarkably, the current J is always zero at $\varphi = \pi$. The temporal asymmetry can control the direction of the current, while the phase shift can only determine the amplitude of the current.

For a narrow symmetric channel with the straight midline ($\varphi = 0$), the channel width $h(x)$ at the bottleneck is $2b$ and the current J is a peaked function of the radius at the bottleneck. Especially, when $b = 0$, the bottleneck is zero. Thus the particles cannot pass through the bottleneck, the current goes to zero [20, 21]. However, for a narrow asymmetric channel with the non-straight midline ($\varphi \neq 0$), the position of the bottleneck not only depends on x but also φ. As φ is increased, the position of the bottleneck moves to the left (Fig. 6).

Figure 7 shows the current J as a function of the channel width b at the bottleneck for different values of φ. When $b \to 0$, the channel is blocked and the particle can not pass from one cell to another, so the current J goes to zero. When $b \to \infty$, the channel reduces to a straight one and the effect of the channel shape disappears. Thus the current J tends to zero. Therefore, there exists an optimized value of b at which the current J takes its maximum value. Note that the peak values of the current move to the left with the increase of φ. It indicates that the current can be manipulated by changing the phase shift φ.

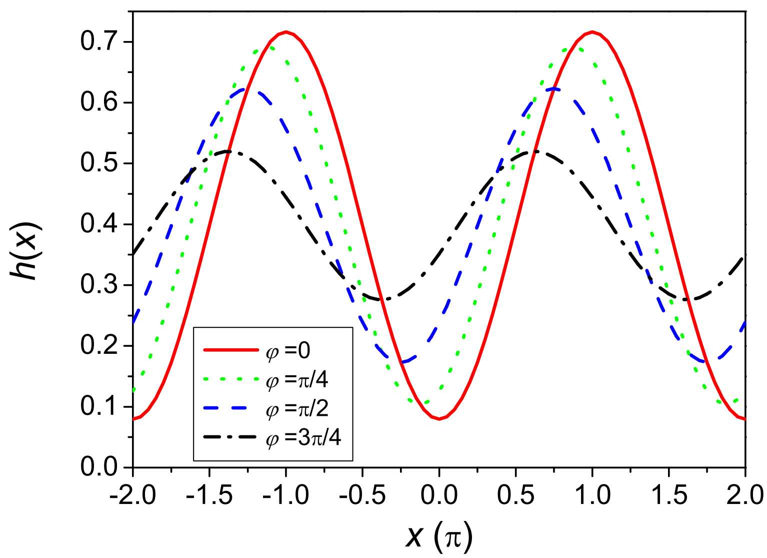

FIG. 6. (color online). Channel width $h(x)$ as a function of x at $a = 1/(2\pi)$ and $b = 0.25/(2\pi)$ for the phase shift $\varphi = 0$ (solid), $\varphi = \pi/4$ (dotted), $\varphi = \pi/2$ (dashed), and $\varphi = 3\pi/4$ (dash-dotted).

Figure 8 shows the current J versus the amplitude F_0 of the unbiased forces for different values of φ. When $F_0 = 0$, namely, there only exists the effect of the entropic barrier, so the current J tends to zero. As F_0 is increased, the current J tends to a certain value. Note that the maximum value of the current decreases with the increase of φ.

IV. CONCLUDING REMARKS

In this paper, we study the transport of overdamped Brownian particles in a 2D channel with the non-straight midline and narrow varying width in the presence of asymmetric unbiased external force. Both the phase shift and the asymmetry of the unbiased force are the two ways to controlling the current. The temporal asymmetric parameter of the unbiased force not only determines the direction of the current but also affects the current amplitude. The current is always positive for $\varepsilon > 0$, zero at $\varepsilon = 0$, and negative for $\varepsilon < 0$. Thus we can obtain the current reversal by changing the asymmetric parameter ε. Remarkably, the current is also manipulated by changing the midline, which can be changed by the phase

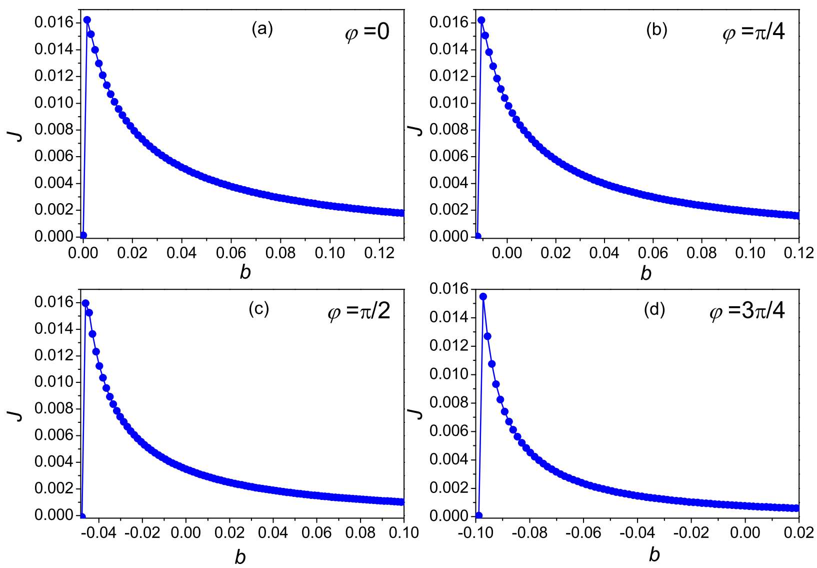

FIG. 7. (color online). Current J as a function of b for different values of φ. (a) $\varphi = 0$. (b) $\varphi = \pi/4$. (c) $\varphi = \pi/2$. (d) $\varphi = 3\pi/4$. The other parameters are $a = 1/(2\pi), k_B T = 0.5$, $\varepsilon = 0.2$, and $F_0 = 1$.

shift between the top and bottom walls of the channel. As the phase shift is increased from 0 to π, the variation of the width decreases and the current also decreases. Especially, the current is always zero at $\varphi = \pi$, this is because the channel width $h(x) = \frac{5}{4\pi}$ at $\varphi = \pi$, the entropic barriers disappear and the ratchet effect also disappears. The results we have presented may have a wide application in many processes, such as transport in zeolites, and nanostructures of complex geometry, controlled drug release, and diffusion in man-made porous materials. In addition, It is very important to understand the novel properties of these confined geometries, zeolites, nanoporous materials, and microfluidic devices, as well as the transport behavior of species in these systems.

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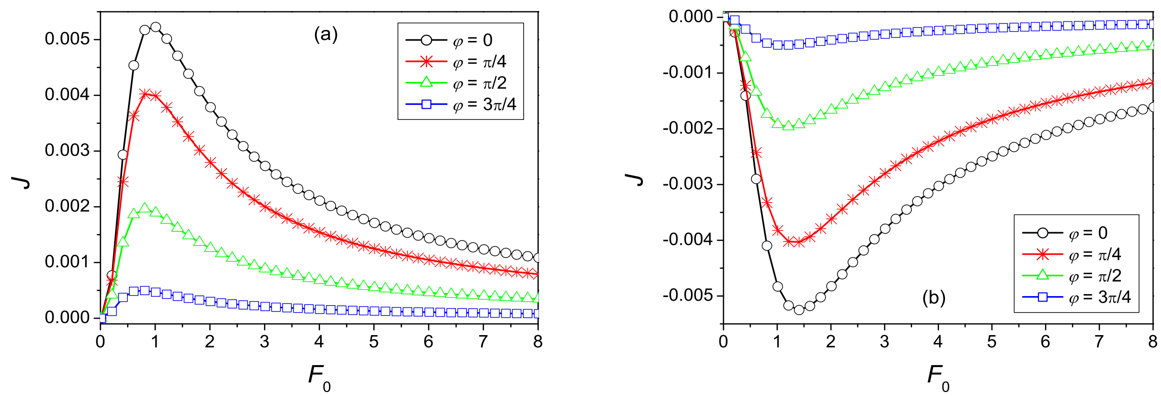

FIG. 8. (color online). Current J as a function of F_0 for different values of the phase shift φ. (a) $\varepsilon = 0.2$. (b) $\varepsilon = -0.2$. The other parameters are $a = 1/(2\pi), b = 0.25/(2\pi)$, and $k_B T = 0.5$.

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