Behaviour of the current in a two-dimensional Büttiker–Landauer motor with entropic barriers*

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The behaviour of the current in a two-dimensional Büttiker–Landauer motor, which is a position-dependent temperature-driven Brownian motor, is investigated in the presence of entropic and energy barriers. It is found that the motion of the Brownian particles is influenced by the shape of the channel. The existence of an entropic barrier can cause an asymmetric current as the flatness ratio of the shape varies. There exists an optimized flatness ratio (nonzero) at which the current reaches its maximum value.

Keywords: Brownian Büttiker–Landauer (BL) motor, entropic barrier, transport properties
PACC: 0540, 0560, 0570L

1. Introduction

Brownian motors are possessed of spatially asymmetric but periodic structures in which the transport of Brownian particles is induced by some nonequilibrium processes, such as the external modulation of the underlying potential or contact with reservoirs at different temperatures.[1−6] A common characteristic of these motors is that they can rectify local spatial or temporal temperature fluctuations into useful work. In recent years, Brownian motors with various forms of energy barriers have attracted much attention. Some authors have studied the energetics and efficiency of Brownian motors.[7−13] Others have investigated the performance of Brownian engines by numerical simulations and molecular dynamic simulations and found them to be in coincidence with the results of theoretical analysis.[14,15] In particular, autonomous thermal engines such as the Feynman–Smoluchowski[16] and Büttiker–Laudauer (BL)[17,18] motors do not require a time-dependent external influence; they are driven solely by thermal fluctuations. Generally, the BL motor is considered to be only an overdamped Brownian particle moving in a periodic potential field, subject to a spatially inhomogeneous temperature. When the temperature changes across a potential barrier, the Brownian particle jumps over the barrier more often from the hot side to the cold side than the other way, and therefore the Brownian particle has a direct motion on average.

The previous work on BL motors was mainly limited to the consideration of energy barriers. However, in some scenarios frequently found in soft condensed matter and biological systems, Brownian particles move in constrained regions such as small pores or channels, whose presence and shape play an important role in their full dynamics.[19−23] In these complex systems, entropic barriers may emerge when a rough description of the dynamics is employed. In this paper, we extend the study of Brownian motors to the case of the existence of both energy and entropic barriers. We investigate the current in a two-dimensional (2D) BL motor with an entropic barrier in the y coordinate axis and an energy barrier in the x coordinate axis, and analyse the effects of the shape of the entropic barrier and the temperature difference on the current of the particles in the motor.

The rest of the present paper is organized in the following way. In Section 2, we introduce our model and develop methods for analysis. In Section 3, we discuss the influence of the temperature difference and the shape of the entropic barrier on the performance of the motor. Finally, we present our main conclusions in Section 4.

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2. Model of 2D BL motor with entropic barrier

We consider Brownian particles moving in a chain of 2D cells (or a 2D channel) aligned in the x axis direction; the structure of the device is shown in Fig. 1.

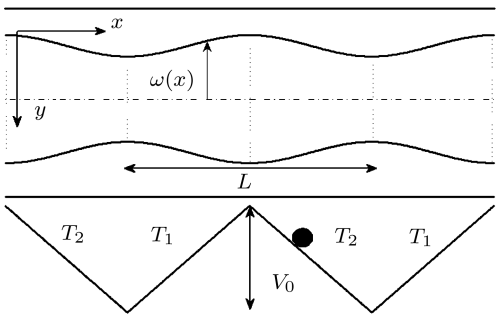


Fig. 1. A chain of two-dimensional cells with entropic and energy barriers. Two reservoirs filled with gas particles at temperatures T_1 and T_2 are alternately connected. Brownian particles (represented by the black circle) are subjected to a piecewise linear potential and may move through the walls. The shape of the chain of two-dimensional cells is determined by its half-width $\omega(x)$.

Each cell has a width that varies in the x axis direction and is filled with gas particles, confined in the cells that they belong to. No direct heat exchange between any two cells through the walls is permitted. The gas particles in each cell act as a heat reservoir with their own temperature, independent of the temperature in other cells. The Brownian particles, unlike the gas particles, are allowed to move freely from one cell to another through the walls, and they are also subject to a potential field $V(x)$, which is periodic in the x axis direction with period L and constant in the y axis direction. For simplicity, we use a piecewise linear potential

$$V(x)=\begin{cases}2V_0x/L, & 0\le x<L/2,\\ 2V_0(L-x)/L, & L/2\le x<L,\end{cases} \tag{1}$$

where V_0 is the height of the potential. In addition to the periodic potential, a constant external force F is exerted on the Brownian particles. We also assume that the temperature is periodic with the same period as that of the potential and is piecewise constant, i.e.

$$T(x)=\begin{cases}T_1, & 0\le x<L/2,\\ T_2, & L/2\le x<L.\end{cases} \tag{2}$$

The shape of the cells is described by their half-width,

$$\omega(x)=-a\cos\left(\frac{2\pi x}{L}\right)+b,\quad 0<x\le L, \tag{3}$$

where a is the parameter that controls the degree of flatness of the cells, and b controls the average half-width of the cells. The widths of the cells at the narrowest and the widest positions are given by $2(b-|a|)$ and $2(b+|a|)$, respectively.

3. Dynamic equations

The dynamics of the suspended Brownian particles here is governed by the Langevin equation,

$$m\ddot{\boldsymbol{r}}=-\gamma\dot{\boldsymbol{r}}-\nabla V(\boldsymbol{r})+F+\sqrt{2\gamma k_{\rm B}T}\boldsymbol{\xi}(t), \tag{4}$$

where $\boldsymbol{r}$ is the two- or three-dimensional position vector, m is the mass of the particle, γ represents the friction coefficient, F is the constant external force, $k_{\rm B}$ is the Boltzmann constant and $\boldsymbol{\xi}(t)$ is the Gaussian white noise, which takes into account ambient thermal fluctuations and is subject to the conditions

$$\begin{aligned}&\langle\boldsymbol{\xi}_i(t)\rangle=0,\\ &\langle\boldsymbol{\xi}_i(t)\boldsymbol{\xi}_j(t')\rangle=\delta_{ij}\delta(t-t'),\quad \text{for}\quad i,j=x,y,z.\end{aligned} \tag{5}$$

In the regime where friction dominates over inertia, the inertial term is usually neglected. The Langevin equation (4) reduces to that in the case of overdamped limit,

$$\gamma\dot{\boldsymbol{r}}=-\nabla V(\boldsymbol{r})+F+\sqrt{2\gamma k_{\rm B}T}\boldsymbol{\xi}(t). \tag{6}$$

When the particles move in a confined medium, their equation of motion can be described by the Fick–Jacobs equation,[24,25] which can be derived from the 2D (or 3D) Smoluchowski equation after integrating over the y (or z) coordinate by assuming equilibrium in the orthogonal direction. The complicated boundary conditions of the equation of motion for an irregular channel can be greatly simplified by introducing an entropic potential that accounts for the reduced space accessible to diffusion for the Brownian particles. Reduction of coordinates may involve the appearance of entropic barriers and an effective diffusion coefficient. When $|\omega'(x)|<1$, the effective diffusion coefficient reads[26]

$$D(x)=D_0\Big/\left[1+\omega'(x)^2\right]^{\alpha}, \tag{7}$$

where $D_0=k_{\rm B}T/\gamma$ is the diffusion coefficient, the scaling exponent α is equal to 1/3 for a 2D channel and the prime refers to the derivative with respect to the spatial variable x.

After the introduction of the entropic potential and the effective diffusion coefficient, Brownian particles moving in a chain of 2D cells (or a 2D channel) may be described by the following equation for the density of particles $\rho(x,t)$:[19−22]

$$\frac{\partial}{\partial t}\rho(x,t) = -\frac{\partial}{\partial x}J(x,t), \tag{8}$$

where J is the particle current, determined by

$$J = -D(x)\frac{\partial\rho(x,t)}{\partial t} - \frac{D(x)}{k_{\rm B}T}\frac{{\rm d}A(x)}{{\rm d}x}\rho(x,t), \tag{9}$$

where $\rho(x,t)$ is the density of particles, $A(x) = E - TS = V(x) - Fx - k_{\rm B}T\ln h(x)$ is the free energy, $E = V(x) - Fx$ is the energy, $S = k_{\rm B}\ln h(x)$ is the entropy and $h(x) = 2\omega(x)/L$ is the dimensionless width.

In the steady state, the density $\rho(x,t)$ is just a function of space and thus the particle current J becomes a constant. The density follows a first-order inhomogeneous linear differential equation, whose formal solution is

$$\rho(x) = \mathcal{Z}(x, c_0, J)\exp\left[-\int_0^x \frac{A'(z)}{k_{\rm B}T}{\rm d}z\right], \tag{10}$$

where

$$\mathcal{Z}(x, c_0, J) = c_0 - J\int_0^x \frac{{\rm d}z}{D(z)}\exp\left[\int_0^z \frac{A'(y)}{k_{\rm B}T}{\rm d}y\right]. \tag{11}$$

The unknown constant c_0 is found by imposing the initial density in the reservoir at temperature T_1, $\rho(0^+) \equiv (b-a)\rho_0$, where ρ_0 is the number of particles per unit width; we then obtain $c_0 = (b-a)\rho_0$. At each wall between cells (at $x = 0, L/2, L$), we must distinguish between particles arriving from the left and from the right, owing to possible discontinuities of temperature. For two cells at different temperatures, the connecting condition is $T_1\rho(0^+) = T_2\rho(L^-)$ and $T_1\rho(L^-/2) = T_2\rho(L^+/2)$.[14]

If the current J is not zero, we must analyse the properties separately in the two cells. From Eq. (10) we have

$$J = \frac{\rho(0^+) - \rho(L^-/2)\exp\left[\dfrac{A(L/2) - A(0)}{k_{\rm B}T_1}\right]}{\displaystyle\int_0^{L/2}\exp\left[\frac{A(z) - A(0)}{k_{\rm B}T_1}\right]\frac{{\rm d}z}{D(z)}} \tag{12a}$$

for $0 \le x < L/2$, and

$$J = \frac{\rho(L^+/2) - \rho(L^-)\exp\left[\dfrac{A(L) - A(L/2)}{k_{\rm B}T_2}\right]}{\displaystyle\int_{L/2}^{L}\exp\left[\frac{A(z) - A(L/2)}{k_{\rm B}T_2}\right]\frac{{\rm d}z}{D(z)}} \tag{12b}$$

for $L/2 \le x < L$.

Because of the complicated form of the effective diffusion coefficient, there is no analytical solution for the particle current J. We therefore analyse the particle current and the particle density in a 2D BL motor by numerical integration of Eqs. (10) and (12) with various parameters.

4. Results and discussion

In this section, we analyse the transport properties of a 2D BL motor for different shapes of the channel and different temperature differences. For simplicity, we take $k_{\rm B} = 1$, $\gamma = 1$, $L = 2\pi$, and $\rho_0 = 10$ for the initial number of particles per unit width, throughout the study. Our method is valid only when $|\omega'(x)| < 1$.

When the temperatures of the cells are different ($T_1 > T_2$), the Brownian particles in the high-temperature cell can reach a higher-potential-energy region than those in the low-temperature cell. Hence, the Brownian particles tend to move across the wall from the hot cell to the cold cell over the potential barrier. At the other wall, the potential is at a minimum and both cold and hot Brownian particles can easily cross to the other side. Therefore, the Brownian particles flow in the positive x axis direction on average. When a force F acting against the direction of motion is added, the motion will slow down and will be stopped when the force is sufficiently large; when the motion is stopped, F reaches the stall force $F_{\rm stall}$. Equation (12) gives the relationship between the external force F and the current J (see Fig. 2).

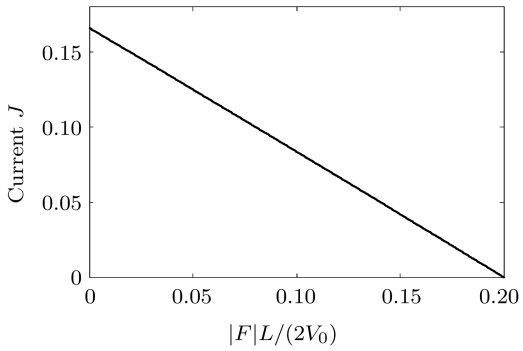


Fig. 2. Current J as a function of the external force F with $V_0 = 1$, $T_1 = 1.5$, $T_2 = 1$, $a = 0.2$ and $b = 0.5$.

When the current J of Brownian particles becomes zero, from Eq. (10) we have

$$\rho(x) = \begin{cases} \rho(0^+)\dfrac{\omega(x)}{\omega(0)} \exp\left[\dfrac{-V(x)+Fx}{k_{\rm B}T_1}\right], & 0 \le x < L/2, \\ \rho(L^+/2)\dfrac{\omega(x)}{\omega(L/2)} \exp\left[\dfrac{V_0 - V(x) + F(x-L/2)}{k_{\rm B}T_2}\right], & L/2 \le x < L. \end{cases} \tag{13}$$

Figure 3 shows the density profiles for two different values of the flatness parameter a as a function of the x coordinate when the current J is zero.

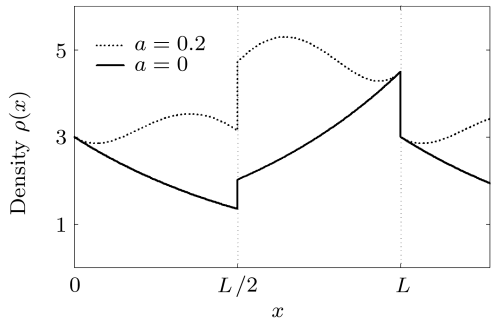


Fig. 3. Distributions of the density $\rho(x)$ for different values of flatness parameter a at $J = 0$; the other parameters are $V_0 = 1$, $T_1 = 1.5$, $T_2 = 1$, $b = 0.5$ and $F = F_{\rm stall}$.

When the shape of the cells is changed by varying a and b, we obtain some novel results. When a is zero (or b is much larger than a), the channel becomes flat and the entropic barrier vanishes, and the current J becomes directly proportional to b (see the solid line in Fig. 4). It can be seen from Fig. 4 that the current J changes much when b is close to a.

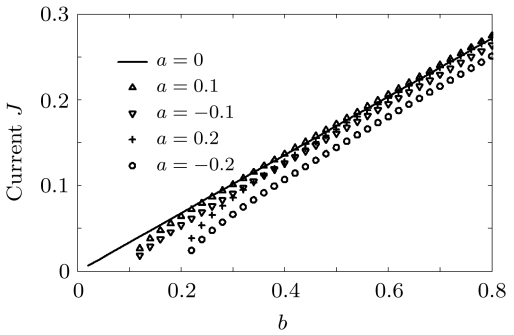


Fig. 4. Current J as a function of b. Other parameters are $V_0 = 1$, $T_1 = 1.5$, $T_2 = 1$ and $F = 0$.

When the temperatures of the cells are equal, the Brownian particles flow from one cell to another in dynamic equilibrium, and no current is produced. As the temperature difference ΔT is increased, the Brownian particles can gain more energy by rectification of fluctuations, thereby leading the current to increase. The existence of an entropic barrier always magnifies the rectification of fluctuations, no matter whether it promotes or hampers the transfer of Brownian particles as shown in Fig. 5.

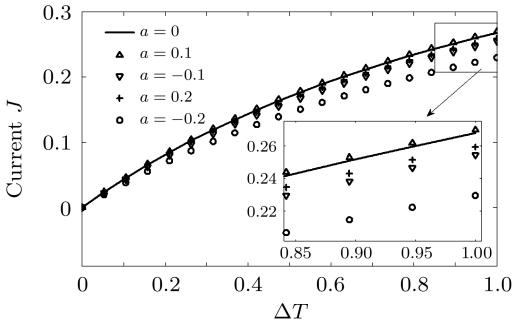


Fig. 5. Current J as a function of temperature difference $\Delta T = T_1 - T_2$. Other parameters are $V_0 = 1$, $T_2 = 1$, $b = 0.5$ and $F = 0$.

A symmetrically shaped channel can lead to an additional flux when the temperatures of the cells are different. If the boundaries between the cells have a spacing of half a period (as shown at the left in Fig. 6), the widths of the walls become different. In the case of positive a (as shown at the top left in Fig. 6), the Brownian particles can gain additional flux because of the increased width of the walls at the position of maximum potential ($x = L/2$). Thus the current of particles in the case of positive a will be larger than that in the case of a negative a by the same magnitude (lower left in Fig. 6); see the solid line in Fig. 7. The current has an asymmetric behaviour with the parameter a/b. When the flatness ratio a/b is equal to $(a/b)_{\rm m}$, the current reaches its maximum value $J_{\max}$. Asymmetry between the widths of the walls at the positions of maximum and minimum potential drives an additional flux with or against the direction of the motion driven by temperature. If the boundaries between the cells have a spacing of one period (as shown at the right in Fig. 6), the widths of the walls are equal. No additional flux is caused by the increased width of the channel at the maximum-potential walls. In this case the current is always lower than that in the case of a flat boundary condition ($a = 0$) as shown by the dot

line in Fig. 7. The entropic barrier always hampers the flow of Brownian particles, both when the boundaries between the cells have a spacing of one period and when they have a spacing of half a period.

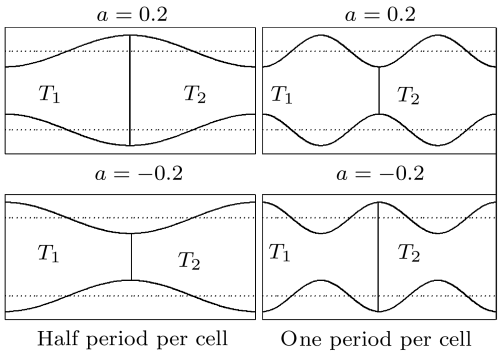


Fig. 6. Schematic diagram of channels with different periodicities.

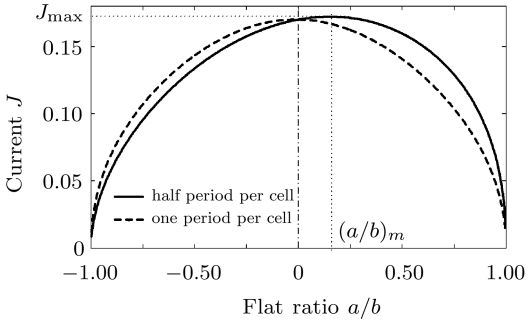


Fig. 7. Current J as a function of flatness ratio a/b. Other parameters are $V_0 = 1$, $T_1 = 1.5$, $T_2 = 1$, $b = 0.5$ and $F = 0$.

5. Conclusions

We present a theoretical study of the relationships between the shape of the channel in a BL motor and the current of Brownian particles for different widths, flatness ratios and temperature differences. In the case of flat boundary, the motor reduces to a 2D chain of cells with a fixed width. In other cases, we must consider both the variation of the width of the walls between the cells and the existence of an entropic barrier caused by the nonzero flatness parameter a. When the temperatures of the cells are different, the temperature difference drives a direct motion from hot to cold cells over the potential barrier. When the width of the channel varies, the density profile of the particles is redistributed. The difference in the width of the channel at the wall between the maximum and the minimum values of the potential causes an additional flux. Meanwhile, the particles will be hampered by an entropic barrier when they flow through the channel. On the whole, the current of Brownian particles has an asymmetric behaviour with the flatness ratio a/b.

Although the model presented here does not match any realistic model, the results that we have presented may provide theoretical guidance to the exploration of the problems of nonequilibrium transportation in BL motors, soft condensed matter, biological systems and nanotechnological systems.

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