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Brownian pump with an unbiased external force

Research Article

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Abstract: We investigate Brownian pump transport in the presence of an unbiased external force. The pumping system is embedded in a finite region bounded by two particle reservoirs. In the adiabatic limit, we obtain the analytical expressions of the current and the concentration ratio. We find that Brownian particles can be pumped through an asymmetric potential from a particle reservoir at low concentration to one at the same or higher concentration in the presence of an unbiased external force.

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Keywords: brownian pump • current • concentration ratio

1. Introduction

Membranes are important to living cells. This is not only because they act as a protective permeability barriers that preserve cells' internal integrity but also because they can control the movement of the necessary materials. Membranes are important in intracellular communications, via the motor proteins incorporated in the cytoskeletal meshwork [1, 2]. Many experiments have been conducted to investigate the roles of motor proteins in particle exchange.

A system with two thermal baths of different temperature can extract mechanical work from the hotter thermal bath. That function has been fulfilled by thermal engines. It is also well known that any object in a thermal bath exhibits random energy fluctuations of the order $k_B T$. These fluctuations are relatively tiny for macroscopic objects but they can not be ignored for nanometric objects such as biological motors: kinesins, dyneins, *etc* [3]. So we naturally hope that some devices that can make good use of such random energy can be designed. Such devices are called Brownian motors (BM). Such speculation is well embodied in Feynman's famous pawl and ratchet model [4]. From then on, an enormous variety of ratchets have been constructed: pulsating ratchets, tilting ratchets, Seebeck ratchets, quantum ratchets, *etc* [5].

Brownian motors have sparked great scientific interest, and have given rise to extensive theoretical and experimental research due to biophysical motivations and potential nanotechnological such as particle pumps and separate devices. Ai and Liu investigated Brownian pumps in nonlinear diffusive media, and found that the superdiffusive regime exhibits an opposite current for low temperature and that the current in a subdiffusive regime may become forbidden for low temperatures and negative for high temperatures [6]. A. Gomez-Marin and J.M. Sancho present a model of a symmetric Brownian motor which changes the sign of its velocity when the temperature gradient is

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inverted [7]. The absence of thermal equilibrium and destruction of the symmetry are the necessary conditions for the ratchet effect to emerge.

We can separate the ratchets into two types: separate devices, and pump mechanisms.

Particle transport has been realized in man-made devices using several variants of the ratchet concept [8–10], and steps have been taken to develop applications. Bader *et al.* [11] have fabricated a silicon-chip ratchet device capable of transporting small DNA molecules in an aqueous solution, with potential to replace the inconvenient gel and polymer solutions required for electrophoresis. Resonant activation in a non-adiabatically driven dissipative optical lattice with broken time symmetry is demonstrated by Gommers *et al.*, and they find that the resonance is produced by the interplay between deterministic driving and fluctuations, and show that by changing the frequency of the driving it is possible to control the direction of the diffusion [12]. Huang *et al.* [13] reported that the separation resolution and speed of micro-fabricated Brownian ratchet arrays for DNA separation can be improved dramatically. Their explanation is that the amount of diffusion required for a ratchet is greatly reduced. Recently, Sancho and Gomez-marin [14, 15] presented a model for a Brownian pump powered by a flashing ratchet mechanism. They aimed to find out what concentration gradient the pump can maintain.

In this paper, we extend Sancho and Gomez-marin's work to the case with an unbiased external driving force. We are especially interested in finding how Brownian particles can be pumped from a particle reservoir at low concentration to one at the same or higher concentration in the presence of an unbiased external force.

2. General analysis

Realistic systems are always subject to external forces. So, let us consider a Brownian pump in an external force field. Assuming the external force $F(t)$, we can easily obtain the Langevin equation:

$$m\ddot{x} = -\gamma\dot{x} - U'(x,t) + \xi(t), \quad (1)$$

where $\xi(t)$ is thermal noise with the usual correlation

$$\langle \xi(t)\xi(t')\rangle = 2\gamma k_B T\delta(t-t') \quad (2)$$

the effect potential $U(x,t)$ is defined as

$$U(x,t) = U_0(x) - F(t)x, \quad (3)$$

where $U_0(x)$ is ratchet potential, $F(t)$ is an external force periodic in time. As molecular motors work in a nanometric space, the friction term dominates and the the inertia term can be discarded. So, we can obtain the following equation in the over-damped regime

$$\gamma\dot{x} = -U'(x,t) + \xi(t). \quad (4)$$

So, the corresponding Fokker-Planck equation for the density of the particles is [16]

$$\frac{\partial}{\partial t}\rho(x,t) = \frac{\partial}{\partial x}\left[U'(x,t)\rho(x,t)\right] + D\frac{\partial^2}{\partial x^2}\rho(x,t) = -\frac{\partial j(x,t)}{\partial x}, \quad (5)$$

where (x,t) is a dimensionless 1+1 space time and $D = \frac{k_B T}{\gamma}$. k_B is the Boltzmann constant, T is the temperature and γ is friction coefficient. The prime stands for the derivative with respect to the space variable x. $j(x,t)$ and $\rho(x,t)$ describe the probability current and the particle concentration, respectively.

From Eq. (5), it is very easy to find that $j(x,t)$ satisfies

$$j(x,t) = -U'(x,t)\rho(x,t) - D\frac{\partial}{\partial x}\rho(x,t). \quad (6)$$

To simplify the problem, we assume that the external force $F(t)$ changes very slowly with respect to t. In other worlds, its period is longer than any other time scale of the system. So there exists a quasi-static state. In the steady state, the concentration can be seen as a function of space and the flux becomes a constant. We note that Eq. (6) is a first order non-homogeneous linear differential equation whose formal solution can be written as

$$\rho(x) = \exp\left[-\int_0^x \frac{U'(z)}{D}dz\right]\left\{c_0 - \frac{j}{D}\int_0^x dz\exp\left[\int_0^z \frac{U'(y)}{D}dy\right]\right\}. \quad (7)$$

The solution has two unknown constants c_0 and j which can be fixed by imposing suitable boundary conditions according to situations that we would like to study. Next we will proceed to get explicit results using a particular model potential.

3. Explicit expressions

In order to get explicit results of Eq. (7), we propose a piecewise-linear triangular potential $U_0(x)$ shown in Fig. 1. It is defined as

$$U_0(x) = \begin{cases} Q\dfrac{x}{\lambda L}, & 0 \le x < \lambda L, \\ Q\dfrac{L-x}{(1-\lambda)L}, & \lambda L \le x \le L, \end{cases} \tag{8}$$

where Q is amplitude of the potential, L is the length of the potential and $\lambda \in (0,1)$ is its asymmetry parameter. $F(t)$ is an unbiased external force and satisfies

$$F(t) = \begin{cases} F_0, & n\tau \le t < n\tau + \frac{1}{2}\tau; \\ -F_0, & n\tau + \frac{1}{2}\tau < t \le (n+1)\tau, \end{cases} \tag{9}$$

where τ is the period of the unbiased force and F_0 is its magnitude.

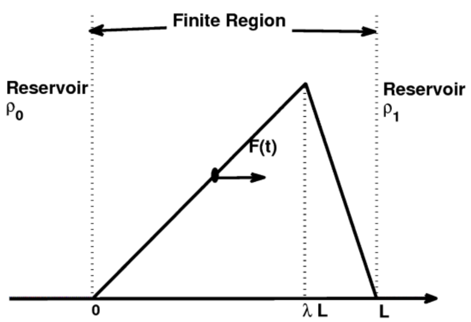

Figure 1. Scheme of a Brownian pump: A spatially asymmetric potential $U_0(x)$(defined in Eq. (8)) is embedded in a finite region and bounded by two particle reservoirs of concentrations ρ_0 and ρ_1. The particles are driven by an unbiased external force $F(t)$, defined in Eq. (9).

According to the boundary conditions given by Fig. 1, the left reservoir concentration $\rho_0 \equiv \rho(0)$ and the right concentration $\rho_1 \equiv \rho(L)$, the unknown constant c_0 in Eq. (7) can be fixed as $c_0 = \rho_0$ and

$$j(F_0) = \frac{D\left\{\rho_0 - \rho_1 \exp\left[-\frac{F_0 L}{D}\right]\right\}}{\int_0^L \exp\left[\frac{U_0(x)-F_0 x}{D}\right] dx} = \frac{D}{I(F_0)}\left\{\rho_0 - \rho_1 \exp\left[-\frac{F_0 L}{D}\right]\right\}, \tag{10}$$

where

$$I(F_0) = \frac{\lambda L D}{Q - F_0\lambda L}\left[\exp\left(\frac{Q-F_0\lambda L}{D}\right) - 1\right] + \frac{D(\lambda-1)L}{Q - F_0(\lambda-1)L}\left[\exp\left(-\frac{F_0 L}{D}\right) - \exp\left(\frac{Q-F_0\lambda L}{D}\right)\right]. \tag{11}$$

The average current is

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

We study the pump capacity using a method similar to that given in Refs. [14, 15]. Pump capacity is usually described by the maximum concentration difference that the pump can maintain between the two particle reservoirs when J tends to zero. Using the condition $J = 0$ and applying Eqs. (10)-(12), we can obtain

$$\frac{\rho_1}{\rho_0} = \frac{I(F_0) + I(-F_0)}{e^{\frac{F_0 L}{D}} I(F_0) + e^{-\frac{F_0 L}{D}} I(-F_0)}. \tag{13}$$

4. Results and discussion

Our study focusses on the current J, and the maximum concentration difference which the pump can maintain when current $J = 0$. For simplicity, we take $k_B = 1$, $\gamma = 1$ and $L = 1$ throughout the analysis.

4.1. Average current

In Fig. 2, we present the current as a function of temperature T. At low temperatures, the particles cannot pass over the potential barrier and the current tends to zero for all densities ρ_1. At higher temperatures, current is higher for lower values of ρ_1. As T increases still further, the ratchet effect disappears: particle transport is dominated by the concentration difference and the particle current reduces and eventually changes direction. There is therefore a region of the operating regime where the current is maximized at finite temperatures; the peak current is greatest, and occurs at a higher temperature, when the concentrations are similar.

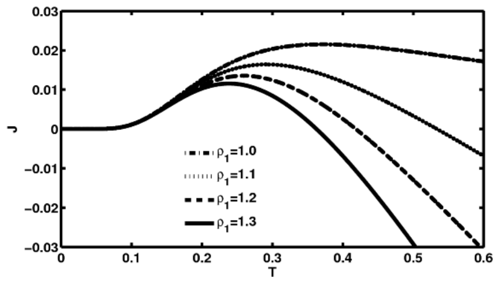

Figure 2. Current J versus temperature T for different values of ρ_1 at $Q = 1$, $\lambda = 0.9$, $F_0 = 0.5$, $\rho_0 = 1.0$ and $\mu = 1$.

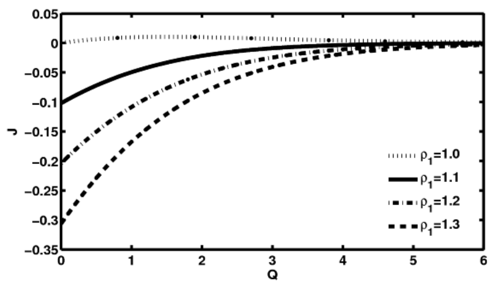

Figure 3. Current J versus amplitude Q for different values of ρ_1 at $T = 1.0$, $\lambda = 0.9$, $F_0 = 0.5$, $L = 1$ and $\rho_0 = 1.0$.

Fig. 3 shows the current J as a function of amplitude of the potential Q for different value of ρ_1. The currents increase with increasing of potential for any fixed ρ_1 and they are negative except for when the concentrations are identical. We can see that the greater the density ρ_1 is, the smaller the current is. When $Q \to \infty$, the particles cannot pass over the potential barrier and the current tends to zero.

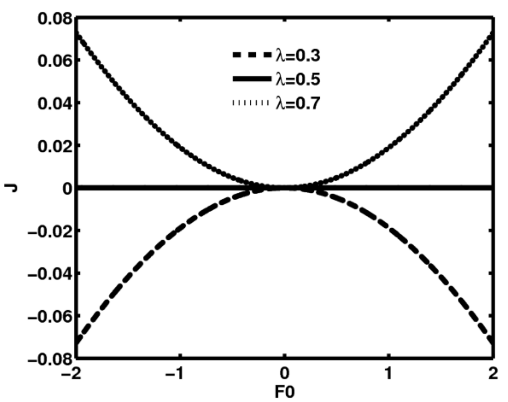

Figure 4. Current J as a function of F_0 for different values of λ at $T = 1$, $Q = 0.9$, $\rho_1 = 1.0$, $\rho_0 = 1.0$ and $L = 1.0$.

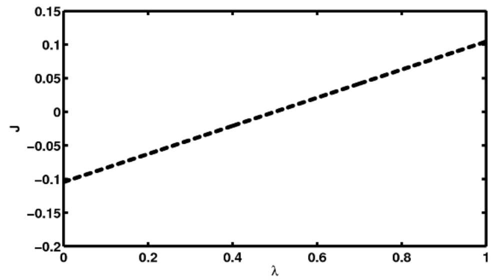

Figure 5. Current J versus λ for $J = 0$ at $Q = 1.0$, $T = 1.0$, $F_0 = 0.5$, $\rho_0 = 1.0$, $\rho_1 = 1.0$ and $L = 1.0$.

Fig. 4 shows the current J versus amplitude of the unbiased external force F_0. We observe that the curve is quite smooth and left-right symmetric for a fixed asymmetry parameter λ. When we take $\lambda = 0.5$, the current disappears for any external forces. The reason for this nil current is that the potential is still symmetric. When the asymmetry parameter $\lambda > 0.5$, the current J is positive or zero for all external force F_0. In this case, there exists a minimal and nil current when the external force $F_0 = 0$. The current at asymmetry parameter $\lambda < 0.5$, contrasted with the above, is negative or zero for all external forces. In this case, the ratchet effect disappears and the particles move to the left. The maximal (and nil) current occurs at the same position, namely when $F_0 = 0$.

In Fig. 5 we illustrate the current J versus the asymmetry parameter λ. We see an increasing linear behavior and the curve is left-right inversion symmetric. Note that when $\lambda = 0.5$, the device does not pump because the spatial symmetry is not broken and there is not a preferred direction. When the asymmetry parameter $\lambda < 0.5$, the current is negative, but for the asymmetry parameter $\lambda > 0.5$, the current is positive, namely, the particles can be pumped from the left reservoir to the right. The more asymmetric the potential, the stronger the system's pumping capacity.

4.2. Concentration ratio ρ_1/ρ_0

Fig. 6 shows the concentration ratio $\rho_1/\rho_0(J = 0)$ as a function of T for different magnitudes of the potential. We note that the smaller the amplitude of the potential is, the larger the concentration ratio is. When $T \to 0$, the concentration ratio $\rho_1/\rho_0 \to \infty$. which means that no particles can pass over the barrier. Increasing temperature T reduces the ratchet effect and decreases the pumping capacity. Surprisingly, the temperature corresponding to the maximum current differs from that at which the concentration ratio for zero current is maximum. This phenomenon can be explained by zero current inducing the maximum

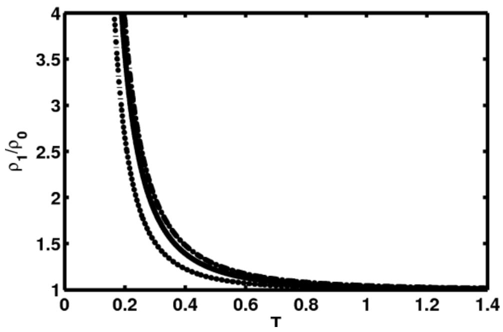

Figure 6. Concentration ratio ρ_1/ρ_0 as a function of temperature T for $J = 0$ at $\lambda = 0.9$, $F_0 = 0.5$, $L = 1.0$ and $Q = 1.0, 2.0, 3.0$.

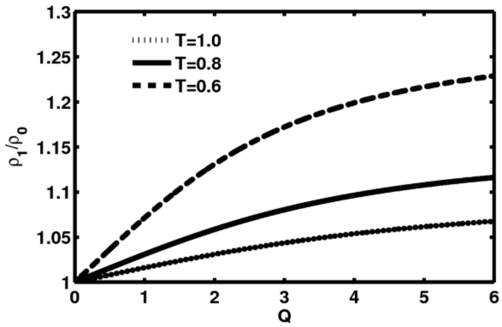

Figure 7. Concentration ratio ρ_1/ρ_0 as a function of Q for different temperature T at $\lambda = 0.9$, $F_0 = 0.5$ and $L = 1.0$.

concentration ratio, not the minimum one.

In Fig. 7, we plot concentration ratio versus parameter Q. At $Q = 0$ there is no concentration difference because no ratchet exists there. Increasing the amplitude of the potential Q leads to an increase of the concentration. For all values of Q, an increase in value of temperature T leads to a decrease in concentration ratio ρ_1/ρ_0. When $Q \to \infty$, the concentration ratio for lower temperature tends to be a certain constant. The reason we given is that influence of the potential barrier can be neglected at the higher temperature.

The concentration ratio as function of the external force F_0 for different values of λ is plotted in Fig. 8. When the asymmetry parameter $\lambda = 0.5$, no matter how large the force is, this device is not able to maintain the concentration difference. The reason for this is that the spatial symmetry is not broken. When the asymmetry parameter $\lambda > 0.5$, the value of concentration ratio ρ_1/ρ_0 is almost above 1 except the point $F_0 = 0$ and increases with increasing $|F_0|$. However, when the asymmetry parameter $\lambda < 0.5$, the device pumps the particles from the right reservoir to the left and the pumping capacity increases with increasing $|F_0|$ too.

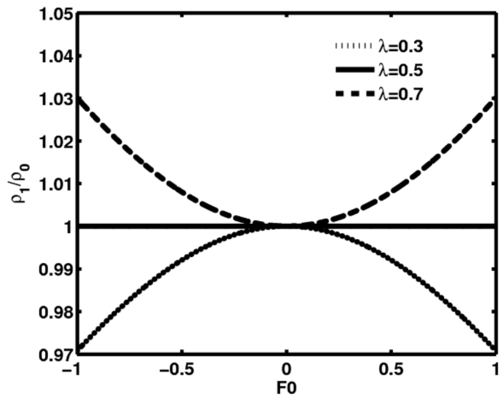

Figure 8. Concentration ratio ρ_1/ρ_0 versus F_0 for different values of λ at $Q = 1$, $T = 1.0$ and $L = 1.0$.

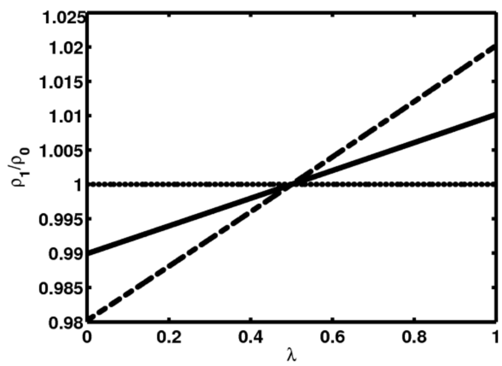

Figure 9. Concentration ratio ρ_1/ρ_0 as a function of λ for $J = 0$ at $T = 1$, $F_0 = 0.5$, $L = 1.0$ and $Q = 0, 0.5, 1.0$.

We also can investigate the concentration ratio ρ_1/ρ_0 as a function of the asymmetry parameter λ and illustrate it in Fig. 9. This figure shows that the curves are right-left inversion symmetric with increasing linear behaviors. All of the lines intersect at $\lambda = 0.5$. In the area (the asymmetry parameter λ is above this point), the right concentration is larger than the left, in other words, the device is able to maintain such concentration difference. However, when the asymmetry parameter $\lambda < 0.5$, the concentration of the right reservoir is smaller than the left, the ratchet effect disappears. Another feature need to be emphasized is that the larger the amplitude of the potential Q is, the larger the concentration ratio is for $\lambda > 0.5$; however, the result for $\lambda < 0.5$ is opposite. When $Q = 0$, for all values of λ the concentration of the right amounts to the left.

5. Concluding remarks

In this work, we have studied a Brownian pump powered by an unbiased external force. The pump is embedded in a finite region and bounded by two particle reservoirs. In the adiabatic limit, we obtain the analytical results for normal diffusion regime and expresses the average current and the concentration ratio as functions of the parameters of the system.

To our surprise, the relationship between concentration ratio and external force is the same as that between average current and external force. Besides, it presents a linear relationship with λ. Another interesting feature deserves our attention too. For high temperature, the efficiency of the ratchet always degrades. However, for low and moderate temperature, the efficiency of the ratchet goes up. So, there is a region around $T = 0.28$ of the operating regime where the efficiency is optimized. In conclusion, to enable the device works well, two conditions—external force and broken symmetry potential—must be met. In other worlds, the ratchet potential and external force affect the operation of the pump.

Another interesting feature would be to analyze the dynamical aspects, such as the pumping flux as a function of time. Though the model dramatically differs from realistic model for biological pumps, the result we have presented contributes to the future investigation in membrane proteins and other realistic pumps. Because one could check that our approach and model allows to enter in the molecular scale in which real pumps do operate, for example the typical energies of order $k_B T$, fluxes, realistic concentration gradients on biological length scales.

Acknowledgements

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