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IMPROVEMENTS OF THE BROWNIAN MOTOR EFFICIENCY

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Abstract: A possible improvement of the directed motion of an inertial Brownian motor should operate on the identification of the optimal conditions that maximize the motor current and minimize its dispersion. In this paper, we have analyzed the role of a bias on the motion of a rocked ratchet in an asymmetric potential making use of a numerical simulation of the inertial Brownian motor. The existence of a critical range for negative loads correpsondent to optimal efficiency for the transport properties of the Brownian motor has been found. In turn, the connection between the load and the efficiency is discussed.

AMS Subject Classification: 60J65
Key Words: inertial Brownian motor, asymmetric potential, numerical simulation

1. Introduction

Molecular motors operate in an environment dominated by viscous friction and thermal fluctuations. The chemical reaction in a motor may produce an active force at the reaction site to directly move the motor forward. The mechanism of generating a unidirectional motion is called the power stroke motor mechanisms [20], [13]. Alternatively, a molecular motor may generate unidirectional motion

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by rectifying thermal fluctuations using free energy barriers established in the chemical reaction. In this one-dimensional motion, if the thermal fluctuations in one direction are blocked, then the motor will be carried forward by thermal fluctuations in other directions. The mechanism of generating a unidirectional motion is called the Brownian ratchet mechanism [14], [2], [3], [5], [16]. Typical examples are rocking ratchets [12], flashing ratchets [7], diffusion ratchets [17], correlation ratchets [4], white-shot-noise ratchets [9] and entropic ratchets [19].

When we study the motion of Brownian motors, the natural transport measure is a conveniently defined asymptotic average velocity of the Brownian motors. It describes how much time the typical particle needs overcome a given distance in the asymtotic time regime. In addition, the quality of the transport and the energetic efficiency play a key role. In this paper, we focus the attention on the accurate usage of the efficiency and its help to define some dynamics properties of the Brownian motor. When a motor is working against a conservative force, the thermodynamics efficiency is well defined as the energy conversion efficiency, which is the ratio of energy output to energy input. This definition is good for both macroscopic motors or molecular motors. Nevertheless, a macroscopic motor does not feel any significant difference between working against the viscous friction and working against a conservative force of the same magnitude. Thus, the effective efficiency comes out by the addition between the energy conversion factor and the so-called Stokes efficiency [10].

In this paper, following the recent proposal of Machura et al, [11], [1], [6], the conditions for optimal conditions for transport properties for inertial Brownian motor moving in an asymmetric potential under a constant load have been analyzed. We found that optimal conditions for transport property of the inertial Brownian motor studied are obtained for negative loads, and that the transport mechanisms are not symmetric for negative or positive loads.

2. Inertial Brownian Motor

An inertial Brownian motor is represented by a classical particle of mass M moving in a spatially periodic and asymmetric potential $V(X) = V(X+L)$ with period L and barrier height V_0. The particle is driven by an external unbiased, time-periodic force of amplitude A and angular frequency Ω. The system is additionally subjected to thermal noise $\eta(t)$. The system can be modelled by the Langevin equation [8]:

$$M\ddot{X} + \Gamma\dot{X} = -U^{'}(X) + A\cos(\Omega\tau) + \sqrt{2\Gamma k_B T}\eta(t) + F, \tag{1}$$

where a dot denotes differentiation with respect to time and a prime denotes a differentiation with respect to the Brownian motor coordinate X. The parameter Γ denotes the Stokes friction coefficient, k_B is the Boltzmann constant and T is the temperature, F denotes an external load force. The thermal fluctuations due to the coupling of the particle with the environment are modelled by a zero-mean, Gaussian white noise, $\eta(t)$, with auto-correlation function $\prec \eta(\tau)\eta(s) \succ = \delta(\tau - s)$ satisfying Einstein's fluctuations-dissipation relation. Upon introducing characteristic lenght scale and time scale, equation (1) can be rewritten in dimensionless form as follows:

$$\ddot{x} + \gamma\dot{x} = -u^{'}(x) + a\cos(\omega t) + \sqrt{2\gamma D}\xi(t) + f \tag{2}$$

with

$$x = \frac{X}{L}; \quad t = \frac{\tau}{\tau_0}; \quad \tau_0^2 = \frac{ML^2}{V_0}; \quad \gamma = \frac{\Gamma\tau_0}{M};$$

$$u(x) = \frac{V(X)}{V_0}; \quad a = \frac{AL}{V_0}; \quad \omega = \Omega\tau_0; \quad D = \frac{k_B T}{V_0}; \quad f = \frac{FL}{V_0},$$

and the zero-mean white noise $\xi(t)$ has auto-correlation function $\prec \xi(\tau)\xi(\tau^{'}) \succ = \delta(\tau - \tau^{'})$. The characterisctic time τ_0 is the time that a particle of mass M needs to cover a distance $L/2$ under the influence of the constant force V_0/L when starting with a zero velocity. For the asymmetric ratchet potential $u(x)$, we consider a linear superposition of two spatial harmonics

$$u(x) = \sin(2\pi x) + \frac{\Delta}{2}\sin(4\pi x), \tag{3}$$

where Δ is the asymmetric strenght of the potential.

The efficiency for the inertial Brownian motor in presence of load and friction does not correspond to purely efficiency of energy conversion. This is so because a direct conversion of energy requires that the energy output for time is described by $f \prec v \succ$ correspondent to the work done against an external force f, while $\prec v \succ$ is the asymptotic average motor velocity, averaged on the initial conditions of positions and velocity and overall realizations of the thermal noise, [10]. In absence of the load force f, such efficiency should be zero. On the contrary, in many cases, such as for protein transport within a cell, the Brwonian motor operates at a zero load force and its goal is to carry a cargo across a viscous environment. As a consequence, the minimal energy input required to move a particle in presence of friction γ over a given distance, depends on the average motor velocity [10]. Combining such requirements, recently, it has been proposed the following efficiency relation [8], [18]:

$$\epsilon = \frac{f \prec v \succ + \gamma \prec v \succ^2}{\gamma(\prec v^2 \succ - D)}, \tag{4}$$

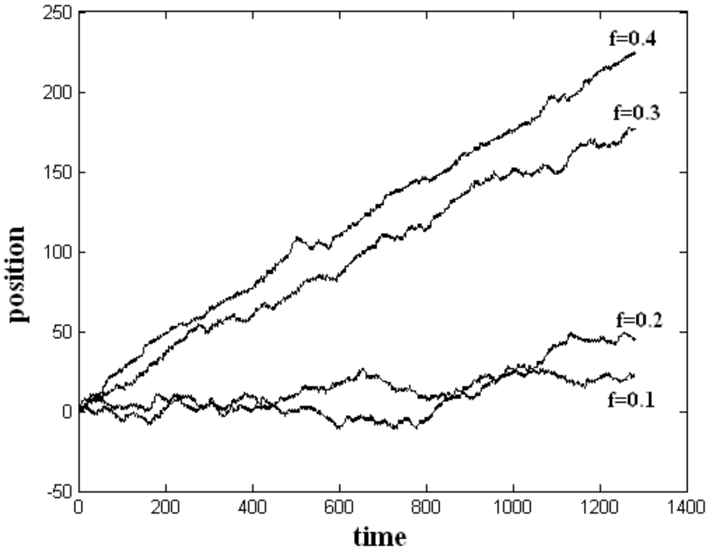
where f, D and γ are the same as defined for equation (2).

3. Numerical Results

Our goal is on finding the behaviour of the asymptotic mean velocity as a function of the load f. The asymptotic mean velocity is defined as the average of the velocity over the time and thermal fluctuations. We have numerically integrated eqaution (2) by the Stochastic Runge-Kutta algorithm of the second order with time step $\Delta t = 0.001$. The initial condition of $x(t)$ was taken from an uniform distribution over the dimensioless period $L = 1$ of the ratchet potential and the initial conditions for the velocity were chosen randomly from a distribution over the interval $[-0.2, 0.2]$. The data obtained were averaged over 32 different trajectories and each trajectory evolved over 10^3 periods. The role of the load was studied analysing its effects both on the trajectories of the Brwonian motor and on the asymtotic mean velocity and efficiency. We have restricted the discussion here to a set of optimal driving parameters, reading a=4.2, ω=4.9, γ =0.9, [11], [6]. The numerical results are synthesised by Figures 1 and 2. Figure 1 shows typical trajectories of the inertial rocking Brownian motor as a function of the sign of the load f, Figures 1 (a) and (c), or as a function of the asymmetric strenght of the potential Δ, Figure 1(b).

Generally, there are two possible dynamical states of the ratchet system: a locked state, in which the particle oscillates mostly within one potential well, and a running state, in which the particle surmount the barriers of the potential. In addition, it is possible to distinguish two classes of running states: in the first one, the particle overcomes the barriers without any back-turns, in the second one, or it undergoes frequent oscillations and back-scattering events. For a small driving amplitude, we find that the locked behaviour is generic, implying thet the average motor velocity is almost zero. If the amplitude is increased up to some critical values, the running solutions emerge. We have explicitly considered only a value over the critical threshold for the driving amplitude. It has been shown that around such critical threshold, the dynamics of the particle is dominated by a complex effects of attractors and the particle burns energy for both barrier crossings and intra-well oscillations. As a consequence, this behaviour is reflected in an enormous enhancement of the effective diffusion [11], [1].

For large value of the asymmetric height barrier of the potential ($\Delta = 0.4$), the transport properties of the Brownian motor is strongly reduced. This a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f=0.2
f=0.1
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time
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200
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0
-50
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400
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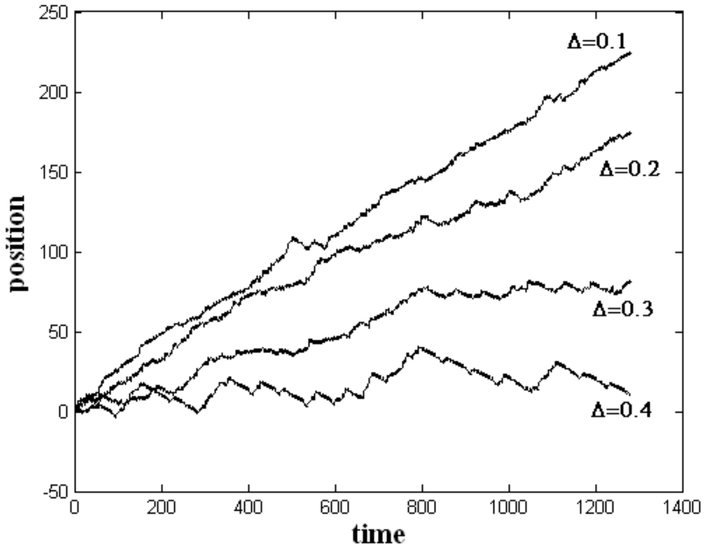
1200
1400

(a)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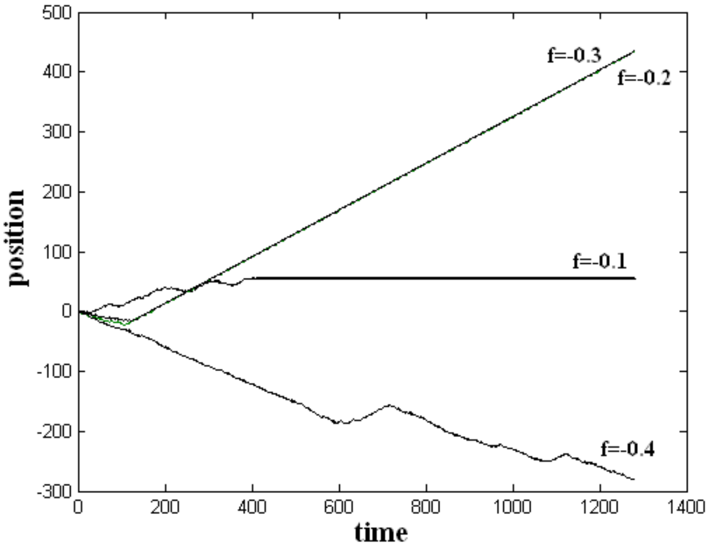
(b)

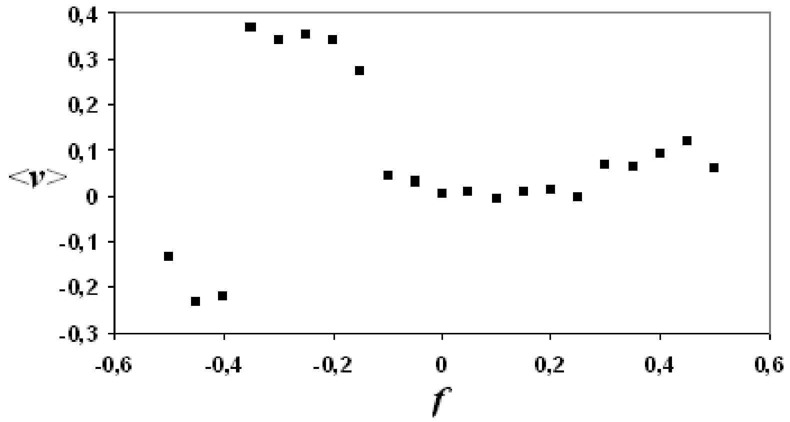
Figure 1



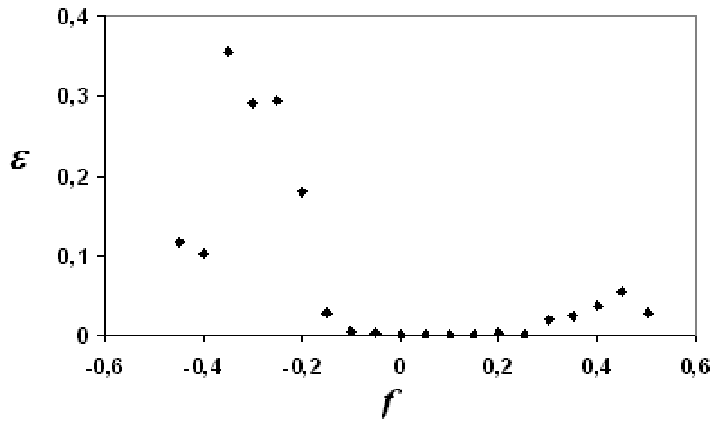
(c)

Figure 1: Continuation: Trajectories of an inertial rocking Brownian motor. (a) A set of different trajectories calculated varying the constant positive load f, with the asymmetric strenght potential taken as $\Delta = 0.1$. Above a critical value of the load ($\succ 0.2$), increasing the load implies the optimization of the transport propertries of the Brownian motor. (b) A set of different trajectories calculated varying the strenght of the asymmetric potential and taking fixed the load ($f = 0.4$). The growth of the asymmetric potential barrier height corresponds to a reduction of the transport properties of the Brownian motor. (c) A set of trajectories for negative loads and with a barrier taken as $\Delta = 0.1$. It is interesting to note that for negative loads, the dynamics of the motor is more complex, two different travel directions can be observed and that the optimal conditions for the transport is obtained for $f = -0.2$ and $f = -0.3$, where the trajectories exactly overlap one each other. Note that the different trajectories in the three plots (a, b and c) are averaged on the 32 different initial conditions. Other parameters are $a = 4.2$, $\omega = 4.9$, $\gamma = 0.9$, $D = 0.001$, in all the three images.

consequence of the growth of the barrier height well of potential that results in an increase of the intra-well oscillations and a more significant quantity of energy gets dissipated per unit distance energy [8].



(a)



(b)

Figure 2: (a) It shows the asymptotic mean velocity as a function of the external force f. (b) The efficiency ϵ as a function of f is shown. The other parameters used were $a = 4.2$, $\omega = 4.9$, $\gamma = 0.9$, and $D = 0.001$. The optimal values of the efficiency were obtained for f comprises between -0.4 and -0.2, at which the mean velocity takes its maximum, indicating that such negative loads facilitate the transport. It is interesting to note the asymmetric role of the load, in fact, we have meanly two local maxima, the higher maximum falls in the range of negative loads.

It is interesting to observe how the asymptotic mean velocity $\prec v \succ$ can represent the transport features showed in Figure 1. Figure 2(a) corresponds to the asymptotic mean velocity as a function of the load f. It shows that the higher values of the velocity are obtained at negative loads, and that such corresponding trajectories are positives, as displayed in Figure 1(c). Otherwise, if we compute the efficiency ϵ as described by equation (4), then the optimal efficiency, $\epsilon \sim 2.8 \div 3.5$ is obtained around $f = -0.35$. Moreover, the asymptotic mean velocity shows three different regimes. Two different transport phases are displayed for negative loads, where the asymptotic mean velocity assumes positive or negative values, and in the case of positive values, the best transport properties are observed. The third one regime was observed for positive loads, such dynamics regime is characterized by rather low mean velocity, and non optimal transport properties. The trajectories show good diffusional properties for values falling around $f \sim 0.4 \div 0.5$. The relevant result of the asymmetric behaviour of the efficiency ϵ as a function of the load is due essentially to an effective reduction of the energy barrier potential, so making more easier transport with respect to positive loads.

4. Conclusions

For improving the directed motion of an inertial Brownian motor, we need to operate on the identification of the optimal conditions that maximize the motor current and minimize its disperison. In this paper, the role of a bias on the motion of a rocked ratchet in an asymmetric potential has been analysed making use of a numerical simulation of the inertial Brownian motor. The existence of a relevant range of negative loads corresponding to optimal efficiency for the transport properties of the Brownian motor has been found.

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