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Isothermal ratchets: Numerical study of the efficiency of the energy transduction

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Abstract

The energetics of isothermal ratchets, that are driven by an external force and operate in contact with a single heat bath, is studied by Langevin equation simulations. The system is analyzed in terms of the mass, friction and amplitude of the external forcing. We found a regime where the efficiency is optimized at finite temperatures, proving that thermal fluctuations facilitate the efficiency of the energy conversion. The condition of optimal efficiency is found, relating mass, temperature and friction to the properties of the ratchet potential. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Much of the interest in non-equilibrium-induced transport processes is concentrated on stochastically driven ratchets [1]. This subject was motivated by the challenge to explain unidirectional transport in biological systems, and several models have been proposed to describe muscle contraction [2], or the asymmetric polymerization of actin filaments responsible of cell motility [3]. More recently, inertial ratchets have been proposed to design molecular shuttles [4], and the model was suggested as a suitable mechanism to describe vesicle transportation in neurons. From a more technological point of view, inertial ratchets have gained much attention in the application to mass separation of Brownian particles [5], or to describe the behavior of electrons in superlattices and Josephson junctions.

While the attention has focused mainly on the measure of the directed current, much less has been done in the characterization of the energetics of the process. To define optimal ratchet models, the maximization of the efficiency of the energy transduction is inevitable.

This topic was first addressed with the introduction of the method of stochastic energetics [6], that was applied to thermal ratchet pumps [7] and to inhomogeneous systems with spatially varying friction coefficient [8]. In both cases, thermal noise was found to facilitate the efficiency of the energy conversion. The behavior of overdamped isothermal ratchets was studied analytically in the quasistatic limit concluding that the efficiency was a decreasing function of the temperature [9]. The effect of thermal fluctuations and inertia on the energetic efficiency of isothermal ratchets, and

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at higher frequencies of the external driving force, remains unknown and is the purpose of the current investigation.

It is known that both current and efficiency do not admit analytic solutions for a general damping or an arbitrary potential. Langevin equation simulation is a simple and effective approach which allow us to calculate, in terms of the mass and damping coefficients, the behavior of the current and the energetic efficiency. The relevance of the results will be discussed in the context of biological systems.

2. The model

The dynamics of a particle of mass μ moving under the influence of an asymmetric potential $V_0(x)$, and subject to an external field $F(t)$, is described by two coupled first-order differential equations:

$$\begin{aligned} \dot{x} &= v, \\ \mu\dot{v} &= -\beta v - \partial_x V_0(x) - \lambda + F(t) + \sqrt{2\beta T}\,\xi(t), \end{aligned} \tag{1}$$

where λ represents an external load against global motion, and β a viscous damping coefficient. $\xi(t)$ is a randomly fluctuating Gaussian white noise with zero mean and autocorrelation function $\langle\xi(t)\xi(s)\rangle = \delta(t-s)$.

We consider $V_0(x)$ to be a piecewise linear but asymmetric ratchet potential of periodicity $L = 1$,

$$V_0(x) = \begin{cases} s_1 x & x \leqslant a, \\ s_2(1-x) & a < x \leqslant L \end{cases} \tag{2}$$

with slopes $s_1 = Q/a$ and $s_2 = Q/(1-a)$. We have fixed $Q = 4$ and $a = 0.75$ throughout the work.

The periodic external driving force $F(t)$ has a square wave form of amplitude A:

$$F(t) = \begin{cases} A, & n\tau \leqslant t < n\tau + \tau_1, \\ -A, & n\tau + \tau_1 \leqslant t < (n+1)\tau. \end{cases} \tag{3}$$

The period τ is assumed to be larger than the time scale of the Brownian particles in the bath environment, but smaller than the diffusion time of the particle over the potential barriers. We have chosen $\tau_1 = \tau/2$, so that $F(t)$ has zero mean.

A quantity of central interest is the time-averaged current J. It can be related to the velocity in the stationary state by $\langle\dot{x}(t)\rangle_{\mathrm{st}} = LJ$, that is directly evaluated from Eq. (1).

The efficiency of the energy transduction η is defined as the ratio between the useful work accomplished by the system in pumping particles against the load λ, and the input of energy that arises from the external driving force. Thus,

$$\eta = \lambda J\tau \left[\int_{x(n\tau)}^{x((n+1)\tau)} F(t)\,\mathrm{d}x(t) \right]^{-1}. \tag{4}$$

We have integrated Eq. (1) by using an stochastic integral algorithm [10], with a time step $\Delta t = 10^{-4}$. Both the current and the efficiency have been averaged over 2×10^4 different trajectories, each trajectory evolving over 75 periods (75τ). We should note that the relative numerical error increases for decreasing β, thus one cannot reach the asymptotic regime $\beta \to 0$.

3. Results and discussions

One of the characteristic features of inertial ratchets is that several reversals in the current are observed depending on the friction strength or mass. We have numerically solved Eq. (1) measuring the current J and the efficiency η as a function of the particle mass at different temperatures. The results for $A = 3$, $\tau = 1$, $\beta = 1$, and $\lambda = 0.01$ are plotted in Fig. 1. There is a temperature above which a positive current is generated for small values of μ, whereas for smaller T the system is dominated by the friction and $J \to 0$. For increasing μ, a region develops where two current reversals take place before the current vanishes due to the weaker effect of the forcing on massive particles. The maximum of the current, for non-negligible inertia, shifts to higher values of μ as T increases, and there is a particular value of the temperature at which the current is maximized, $J_{\max}$, as is shown in the inset plot of Fig. 1.

This behavior is characteristic of a stochastic resonance-like effect and is particularly interesting for the study of voltage-sensitive ion channels. Stochastic resonance has been observed in the measurement of ion current in cell membranes [11], and the problem of ion selectivity could be understood due to a mass sensitivity of the channeled ions.

In Fig. 2 the efficiency is plotted as a function of the temperature for selected values of μ. The maximum of

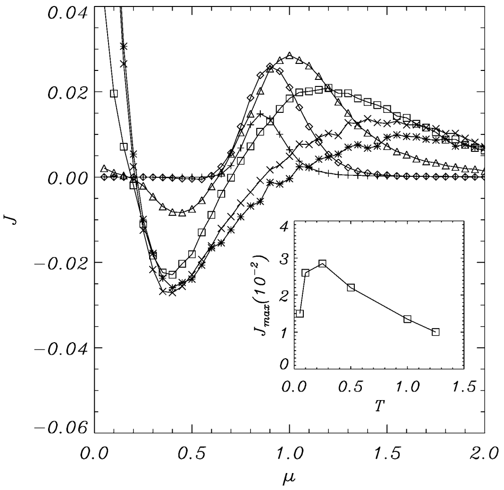

Fig. 1. Current as a function of μ for a viscous damping $\beta = 1$ at temperatures: $T = 0.05$ (+); $T = 0.10$ (⋄); $T = 0.25$ (△); $T = 0.50$ (□); $T = 1.0$ (×); $T = 1.25$ (∗). Inset: maximum current at each temperature.

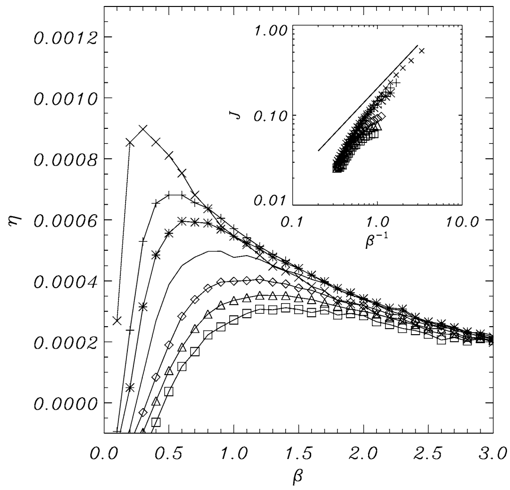

Fig. 3. Efficiency as a function of β, for inertia values: $\mu = 0.01$ (×); $\mu = 0.025$ (+); $\mu = 0.035$ (∗); $\mu = 0.05$ (−); $\mu = 0.07$ (⋄); $\mu = 0.085$ (△); $\mu = 0.1$ (□). Inset: log–log plot of the current vs. β^{-1}. A solid line of slope 1 is included to guide the eye.

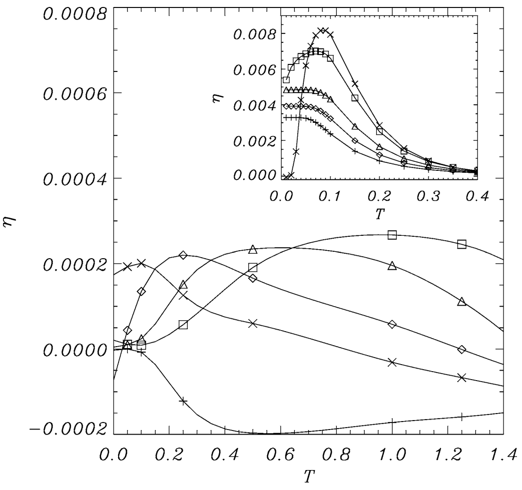

Fig. 2. Efficiency vs. T for a forcing amplitude $A = 3$ and period $\tau = 1$, at inertia values: $\mu = 0.4$ (+); $\mu = 0.8$ (×); $\mu = 1.0$ (⋄); $\mu = 1.3$ (△); $\mu = 1.6$ (□). Inset: overdamped regime ($\mu \to 0$) at $\tau = 50$ and amplitudes: $A = 1.0$ (×); $A = 1.3$ (□); $A = 2.0$ (△); $A = 2.5$ (◇); $A = 3.0$ (+).

the efficiency, located at non-zero temperatures, indicates that thermal fluctuations facilitate the efficiency of the energy conversion. The limiting case of $\mu \to 0$, shown in the inset of Fig. 2, corresponds to a ratchet operating in the overdamped regime. We have selected a much longer period, $\tau = 50$, and the efficiency is evaluated at different amplitudes of the forcing. For small amplitudes the maximum of η is found at $T > 0$, confirming the contribution of the thermal fluctuations to the efficiency. For larger values of A the efficiency is a decreasing function of the temperature having its maximal value λ/A at $T = 0$. This result is in agreement with the theoretical findings of a ratchet system in the quasistatic regime [9].

The effect of the viscosity is studied for different values of μ at $T = 1$, the rest of the parameters being the same as before. For large β, friction dominates and the current drops to zero. On the other hand, for small β, in the strongly underdamped regime, the motor becomes too weak to work against the load force and a negative current is observed. At intermediate β values, the current has a maximum whose location depends on μ. The efficiency, with a similar behavior, is plotted in Fig. 3.

For small μ and large β we fall into the overdamped regime where molecular motors are known to operate. Despite protein friction between motor and filament is expected to be orders of magnitude larger than the viscosity of the solution, an increase of the solvent viscosity is found to decrease the chemical reaction kinetics, strongly influencing the dynamic sliding of the filaments. The shortening of the velocity is found experimentally to be proportional to the solution

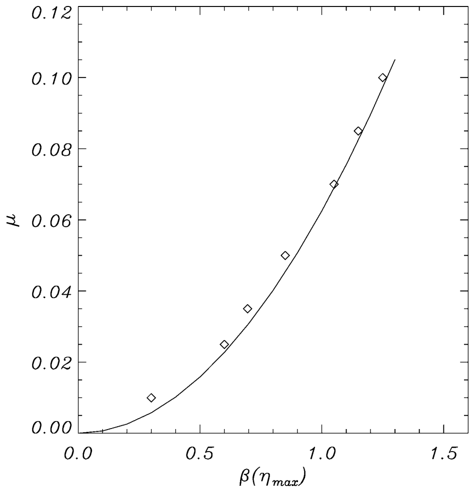

Fig. 4. Damping values that maximize the efficiency vs. the inertia. The data is fitted according to Eq. (5).

viscosity [12]. This linear relationship is also observed in this regime and it is shown in the inset plot of Fig. 3.

For increasing μ the maximum of the efficiency shifts to higher values of β (Fig. 3). This behavior can be easily explained. Due to the spatial asymmetry of the potential, the efficiency of the process can arrive at its optimal value being the particle in a local minimum of the potential and diffusing through a distance, within the characteristic velocity relaxation time μ/β, equal to the width of the hard side of the potential $L-a$. Since the diffusion is given by the ratio T/β, the condition of optimal efficiency can be written as:

$$\sqrt{\frac{T\mu}{\beta^2}} = L - a. \tag{5}$$

The friction values that give the maximum values of the efficiency $\eta_{\max}$ at different μ are plotted in Fig. 4. The data has been fitted according to Eq. (5), with reasonable agreement.

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