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# Optimal efficiency condition and current reversals in forced underdamped ratchets

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**Abstract**

The condition of optimal efficiency in the energy transformation of a massive Brownian particle, moving in an asymmetric potential and subject to an external driving force, is studied by direct simulation of the stochastic differential equations. We analyze the behavior of the stationary averaged current and, at the same time, the energetic efficiency is evaluated. We found that the current exhibits several reversals when plotted as a function of the mass, and that it can be optimized at a particular value of the temperature. The condition to achieve an OPTIMAL EFFICIENCY IS found, relating the 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

In the last years, a large variety of ratchet models have been proposed to study the transport properties of non-linear systems that can extract usable work in the presence of unbiased non-equilibrium forces (for reviews, see [1]). Much of the work was stimulated by its role in describing the physics of molecular combustion motors, and most of it concentrated just on overdamped systems. In these systems, the

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damping coefficient is absorbed into the time scale and also temporal symmetry is applied. However, only recently the effect on the transport of a finite inertia, either in classical [2–7] or quantum [8,9] systems, or an inhomogeneous friction [10,11], has been considered.

The study of classical non-equilibrium underdamped models has gained much interest due to potential novel technological developments such as nanoscale devices that separate Brownian particles in the absence of macroscopic gradients at different friction strength or mass [12], and it has been recently observed in excited granular media [7]. It might be of relevance to the study of intracellular transport as well [13]. In neurons, while the enzyme kinesin moves along microtubules in fast anterogade axonal transport, dynein moves membranous organelles in the retrograde direction [14]. The direction of the carriers is believed to be determined by their geometry, the substrate asymmetry and unavoidable inertial effects [3].

While attention on inertia ratchets has focused on the measure of the directed current, much less has been done on the characterization of the energetics of the process. On the other hand, the maximization of the efficiency has become an important criterion to define optimal models.

The purpose of the present work is to investigate the condition to achieve an optimal efficiency and to study the role of friction and temperature on the direction of current.

We have considered a model consisting of a massive particle moving in an asymmetric periodic potential and subject to a time periodic deterministic driving force of zero average. By performing Langevin equation simulations we have analyzed, in terms of the mass, friction and amplitude of external forcing, the behavior of the current and have measured the efficiency of the energy transformation. We found that the current exhibits several reversals when plotted as a function of the mass and that it can be optimized at a particular value of the temperature. We found a regime where the efficiency is optimized at non-zero temperatures, proving that thermal fluctuations facilitate the efficiency of the energy conversion in forced underdamped ratchets. The condition of optimal efficiency is found relating the mass, temperature and friction to the properties of the ratchet potential.

## 2. The model

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

$$\dot{x} = v \, ,$$

$$\mu\dot{v} = -\beta v - \frac{\partial}{\partial x} V_0(x) - \lambda + F(t) + \sqrt{2T\beta}\,\xi(t) \, , \tag{1}$$

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

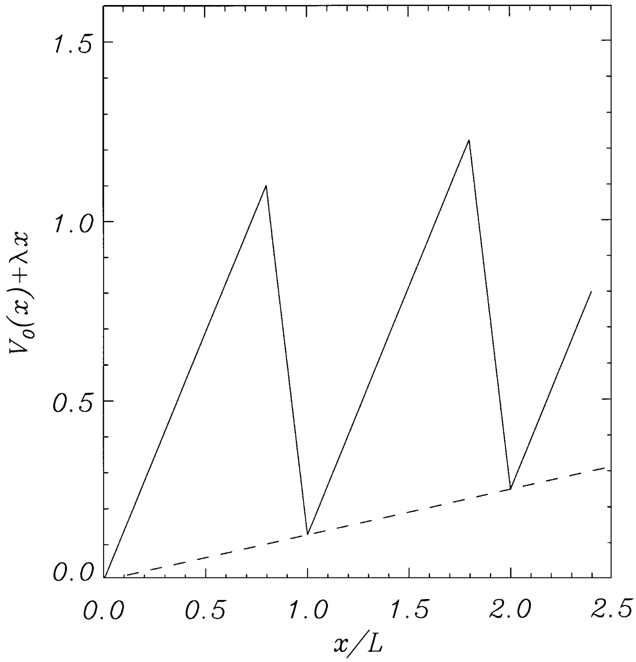



Fig. 1. Schematic representation of the ratchet potential with an additional external load. The dashed line represents the load term $\lambda x$.

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 $s_2 = Q/(1-a)$. Throughout the work, $Q = 4$ and $a = 0.75$. A schematic representation of the potential, including the load term, is shown in Fig. 1.

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 $\tau$ 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. Throughout the paper we have chosen $\tau = 1$ and $\tau_1 = \tau/2$ so that $F(t)$ has zero mean.

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

To obtain the efficiency of the energy transformation, we followed the method of stochastic energetics introduced by Sekimoto [15], previously used in the context of overdamped ratchet systems [16–19]. The efficiency $\eta$ is defined as the ratio of the useful work accomplished by the system in pumping particles against the load force $\lambda$ to the input of energy that arises from the external driving force. Thus,

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

It can be easily proved that the above expression is the same one that holds for the overdamped case [15]. We should notice that for $\mu \to 0$ and $\beta = 1$ we recover the previously investigated overdamped situation [17].

We have integrated Eq. (1) by using a stochastic integral algorithm [20], with a time step of $\Delta t = 10^{-4}$. Both the current and the efficiency have been averaged over $2 \times 10^4$ different trajectories, each trajectory evolving over 75 periods ($75\tau$). We should note that the relative numerical error increases for decreasing $\beta$. Thus one cannot reach the asymptotic regime $\beta \to 0$. We should remark that in the cases studied, the statistical error is small and comparable to the symbol size in all the figures presented.

## 3. Results and discussions

### 3.1. Optimal efficiency condition

In underdamped ratchet models, the friction strength and mass are the most relevant parameters in order to investigate the inertial effects on the transport properties. We will focus first on the dependence of the current and the efficiency on the viscous damping $\beta$ for different values of $\mu$. The rest of the parameters are fixed to $\lambda = 0.01$ and $T = 1$. In order to select a proper amplitude for the external forcing, we first analyze the behavior of the efficiency for an intermediate friction value of $\beta = 0.5$. The results are presented in Fig. 2. From the plots, it is clear that both the current and the efficiency can be maximized with respect to $A$. Small amplitudes compared to the force derived from the ratchet potential are always preferred for having a better efficiency, while for amplitudes large enough, the particle is able to jump over the potential barrier in any direction with equal probability and the ratchet effect becomes almost inefficient. $A = 3$ is close to the one that gives an optimal efficiency in the range of $\mu$ studied, and will be the value selected for the following simulations.

The behavior of the current and efficiency as a function of $\beta$ is represented in Fig. 3. We observe that for small values of $\beta$, in the strongly underdamped regime, the current becomes negative. In this regime, the motor is too weak to work against the load force. At intermediate $\beta$ values the current shows a maximum whose position depends on $\mu$ and, for increasing friction, the current drops to zero. In the latter case, we fall into the overdamped regime where biological molecular motors are known to operate. In this context, it is known that even though protein friction between motor and filament is expected to be orders of magnitude larger than the viscosity of the solution [21], an increase in the solvent viscosity is found to decrease the chemical reaction kinetics, strongly influencing the dynamic sliding of the filaments [22]. For instance, muscle contraction can be easily controlled by adding a solution of low molecular

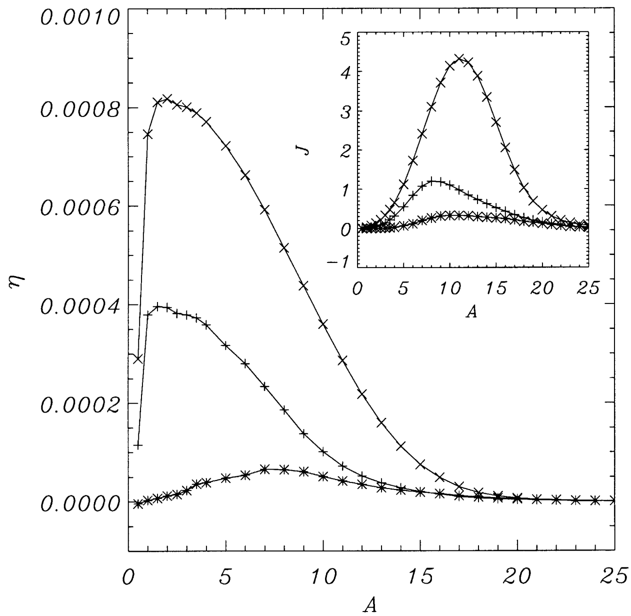


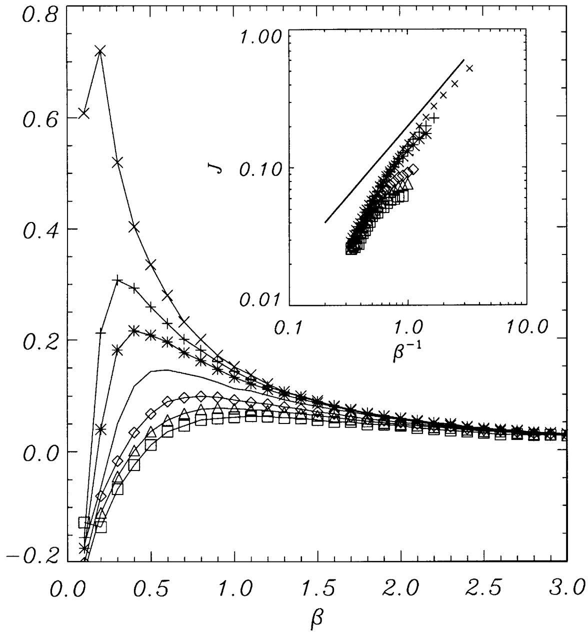

Fig. 2. Efficiency as a function of $A$, at $T = 1$ for different values of the mass: $\mu = 0.01$ ($\times$); $\mu = 0.05$ ($+$); $\mu = 0.1$ ($*$). Inset plot: corresponding current.

weight sugars that increases the viscosity within the myosin filaments. The shortening of the velocity is found experimentally to be proportional to the solution viscosity [23]. We have represented $J$ vs. $\beta^{-1}$ in the inset plot of Fig. 3a. It is remarkable that a linear relationship is recovered for $\mu \to 0$ in agreement with the experimental findings.

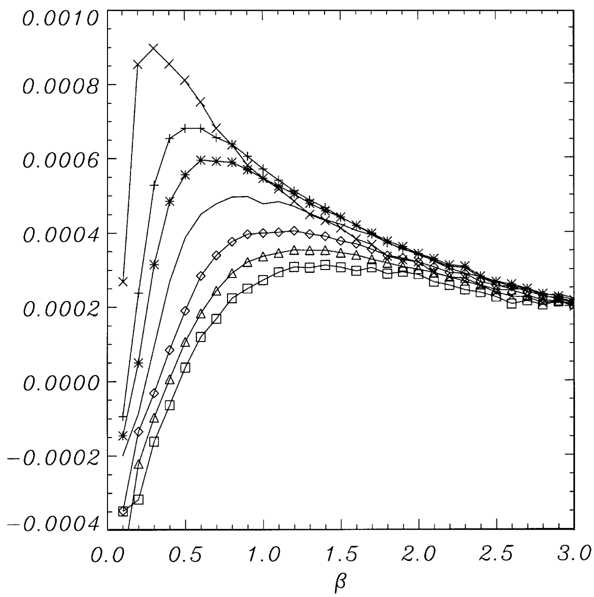
The efficiency, plotted in Fig. 3b, follows the same type of behavior as that observed for the current. We observe that for increasing $\mu$ the maximum in the efficiency shifts to higher values of $\beta$. This behavior will serve to establish a condition for the optimal efficiency. We can define a characteristic velocity relaxation time from Eq. (1): $\tau = \mu/\beta$. On the other hand, the diffusion coefficient is connected to the viscous friction coefficient through the fluctuation–dissipation theorem: $D = T/\beta$. Thus, a particle, within a time interval $\tau$, will travel a characteristic distance $\xi = \sqrt{D\tau}$. Due to the spatial asymmetry of the potential, the efficiency of the process can achieve its optimal value, which is the characteristic distance $\xi$ equal to the width of the hard-side of the potential $L - a$. Therefore, the condition for 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 $\mu$ can be extracted from Fig. 3b and are plotted in Fig. 4. The data have been fitted according to Eq. (5), with reasonable agreement.




(a)




(b)

Fig. 3. (a) Current as a function of $\beta$, for different values of the mass: $\mu = 0.01$ ($\times$); $\mu = 0.025$ ($+$); $\mu = 0.035$ ($*$); $\mu = 0.05$ ($-$); $\mu = 0.07$ ($\Diamond$); $\mu = 0.085$ ($\triangle$); $\mu = 0.1$ ($\Box$). Inset: log–log plot of the current vs. $\beta^{-1}$. A solid line of slope 1 is included to guide the eye. (b) Corresponding efficiency.

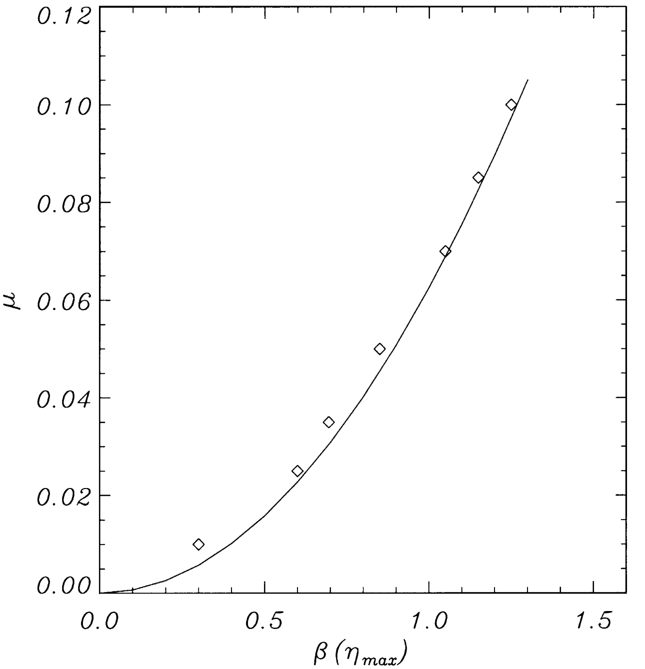



Fig. 4. Plot of friction $\beta$ that gives the maximum values of efficiency as a function of inertia. The data are fitted according to Eq. (5).

It is also interesting to plot the isolines for different efficiency values in the parameter space of $\mu$ and $\beta$ obtained from Fig. 3b. The results are presented in Fig. 5 together with the curve of maximal efficiency.

### 3.2. Mass separation

The dependence of the current $J$ and the efficiency $\eta$ on the particle mass $\mu$ is shown in Figs. 6 and 7. We have taken several values of the friction $\beta$ and present the results at two different temperatures: Fig. 6 is at $T = 0.25$ and Fig. 7 is at $T = 1.0$. The common parameters are $\lambda = 0.01$ and $A = 3$. A nonmonotonic behavior of the current and the efficiency as a function of $\mu$ is clearly illustrated in the figures. We observe the role of the ratchet becoming weak in two limiting cases: (i) for $\mu \to 0$ at low temperatures and (ii) for non-negligible inertia. While in the first case friction dominates, in the second one it is the forcing that has a weaker effect on a larger mass, and thus a decrease of the average velocity is expected.

For small $\mu$ a negative current appears, and with increasing mass a reversal in the direction takes place until a global maximum is reached. After the maximum in the current is reached, the curves decay to zero with the characteristic velocity relaxation time $\mu/\beta$. Note that a smaller value of $\mu/\beta$ corresponds to a larger average current. As

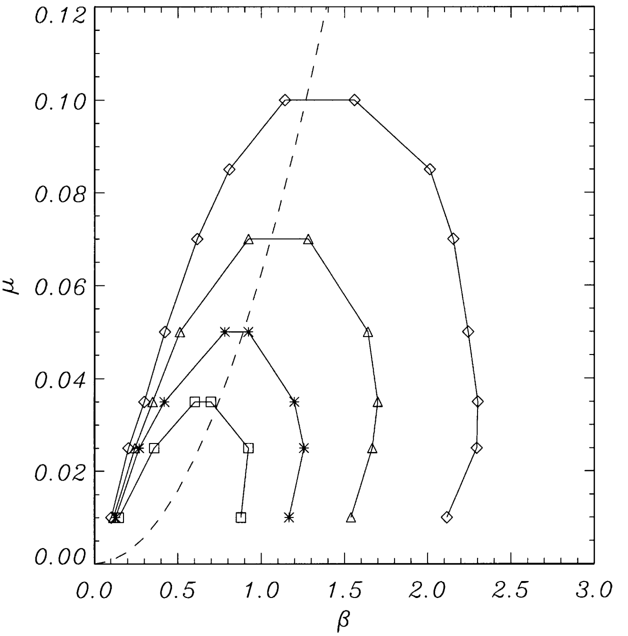


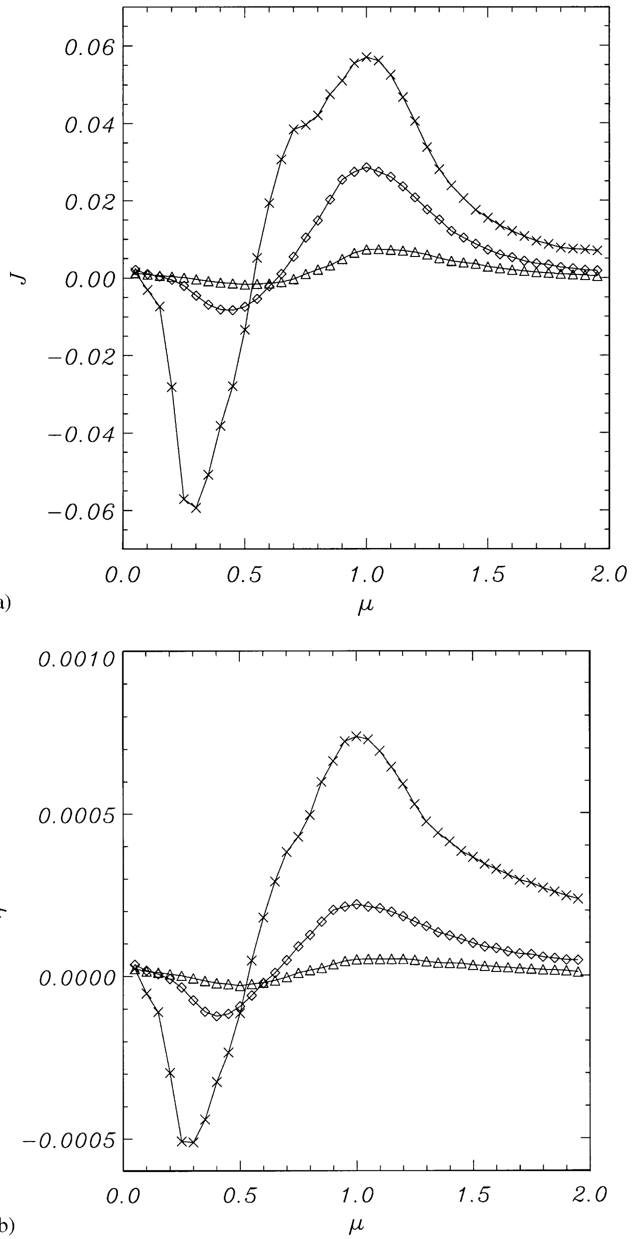

Fig. 5. Contour of the average efficiency in the parameter space of friction and inertia. The different curves correspond to: $\eta = 0.0003$ (◇); $\eta = 0.0004$ (△); $\eta = 0.0005$ (∗); $\eta = 0.0006$ (□). The dashed line corresponds to the line of maximal efficiency.

a consequence, particles should move in different directions according to their masses falling in the two characteristic regimes. This may serve the purpose of separating mesoscopic particles with different masses.

Similar results have been reported when current is plotted as a function of correlation time in ratchet systems that include a source of colored noise [3,5]. The peculiarity of such systems is that breaking the reflection symmetry of the potential is not necessary to obtain a directed transport. A rather different behavior is observed in systems that are driven by a temperature modulation where the current is found to be a monotonic decreasing function of $\mu$ [24].

Curves for the corresponding measured efficiency follow the same type of behavior observed in the current.

In order to show more clearly the effect of temperature on ratchet behavior, we present in Fig. 8 the current and efficiency as a function of $\mu$ for a fixed viscous damping coefficient $\beta = 1$. From Fig. 8a it is clear that there is a temperature above which a positive current generates for small values of $\mu$. For increasing $\mu$, a region develops where several current reversals take place before it vanishes for a large enough $\mu$. It is interesting to note that the global maximum of the current for non-negligible inertia shifts to higher values of $\mu$ as the temperature increases. We also observe that 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. 8a. This behavior is characteristic of a stochastic




(a)

(b)

Fig. 6. (a) Current as a function of $\mu$ at temperature $T=0.25$, for different values of the friction: $\beta=0.5$ ($\times$); $\beta=1.0$ ($\diamond$); $\beta=1.5$ ($\triangle$). (b) Corresponding efficiency.

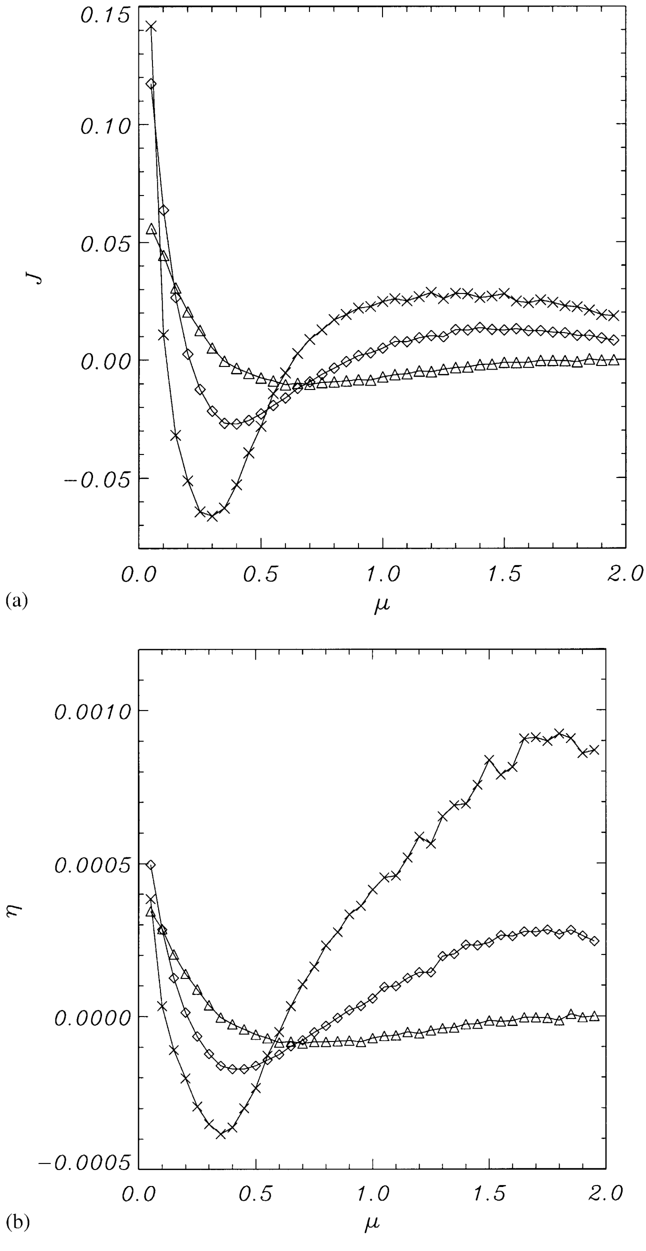
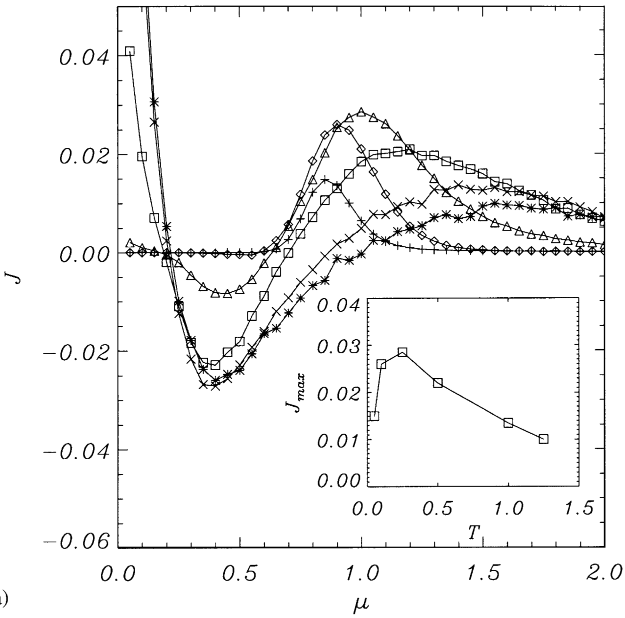
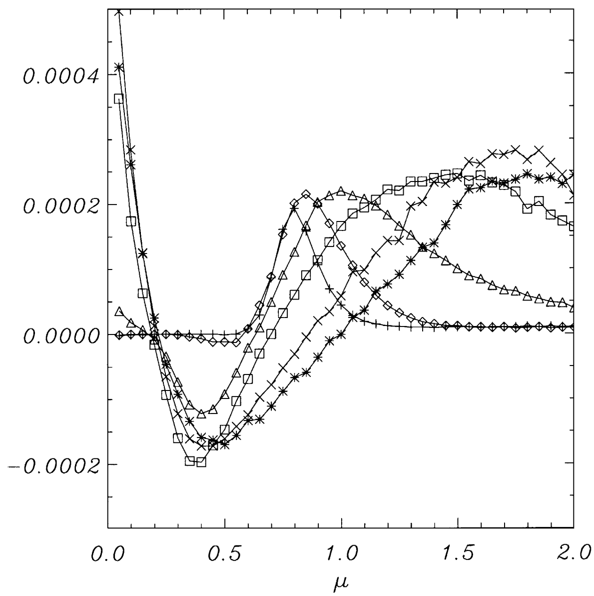



Fig. 7. (a) Current as a function of $\mu$ at temperature $T = 1.0$, for friction values: $\beta = 0.5$ ($\times$); $\beta = 1.0$ ($\diamond$); $\beta = 2.0$ ($\triangle$). (b) Corresponding efficiency.




(a)




(b)

Fig. 8. (a) Current as a function of $\mu$ for a viscous damping $\beta = 1$ and 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. (b) Corresponding efficiency.

resonance-like effect, which is the noise intensity parametrized through the temperature. This result is particularly interesting in the study of voltage-sensitive ion channels [25]. Stochastic resonance has been observed in the measurement of ion current in cell membranes [26]. Moreover, the problem of ion selectivity could be understood due to mass sensitivity of the channeled ions.

Similar behavior is observed in the efficiency. We should note that the efficiency can be optimized at non-zero temperatures, proving that thermal fluctuations may facilitate the efficiency of energy conversion. The maximum of the efficiency takes place at higher values of $T$ when compared with the maximum in the current, indicating that the conditions for obtaining optimal current and efficiency are different. This effect has also been noted in earlier studies on overdamped systems [10,11,19].

## 4. Summary and conclusions

Extensive Langevin equation simulations have been reported in this paper to investigate the energetics of an underdamped forced ratchet. Both the current and the efficiency have been measured as a function of mass $\mu$, friction $\beta$ and amplitude of the external driving force $A$, at different temperatures.

We have provided physical arguments that determine the condition of optimal efficiency, relating mass, temperature and friction to the properties of the ratchet potential. This condition is found to be in agreement with the numerical integration of the stochastic differential equations.

We have found a regime where the efficiency is optimized at finite temperatures, proving that thermal fluctuations facilitate the efficiency of energy conversion in forced underdamped ratchets.

The current is found to exhibit several reversals when plotted as a function of the mass. This result might be of relevance in the development of novel technological applications that may pump or separate Brownian particles in periodic structures. We have observed that the current can be maximized at a particular value of the temperature. The temperature is the tuning parameter that controls the noise intensity, and the observed effect is characteristic of a stochastic resonance process. This result could be of interest in the study of the behavior of ion channels.

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