M.Sc. Physics of Complex Systems

Statistical Physiscs for Biological Systems

Efficiency optimization in forced ratchets due to thermal fluctuations

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Review: Efficiency optimization in forced ratchets due to thermal fluctuations

Abstract

This report is a review of the paper produced by K. Sumithra[1] and T.Sintes[2] in 2001 [1]. The results found by K. Sumithra and T. Sintes about an optimal efficiency in forced ratchets due to thermal fluctuations, that contradict previous results [2], are recovered in this review, giving further support to this contradiction.

1 Introduction

The effect of thermal noise is known to be symmetric for Brownian particles at equilibrium, even in an anisotropic medium. The second law of thermodynamics requires this: Structural features alone, no matter how cleverly designed, cannot bias Brownian motion. However, non equilibrium fluctuations can bias the Brownian motion of particles in an anisotropic medium without thermal gradients, a net force such as gravity or a macroscopic electric field. This bias of the Brownian particles lead to unidirectional transport, which can be interpreted as effective work. A really good and detailed review about this topic can be found in [3].

The development of this subject has been motivated, for instance, by the challenge to explain unidirectional transport in biological systems, which is precisely the reason of this review. A fundamental question one can ask himself is if this procedure can be optimised or, equivalently, if it is optimised in biological systems. O. Magnasco studied the temperature dependence of the current and showed that the current can be maximised at finite temperatures. He claimed that there is a region of operating regime where the efficiency can be maximised at finite temperatures and the existence of thermal fluctuations facilitate the efficiency of energy transformation [1][4]. Later on, Hideki Kamegawa, Tsuyoshi Hondou, and Fumiko Takagi (KHT) conclude that the efficiency of energy transformation cannot be optimised at finite temperatures and that the thermal fluctuations do not facilitate it. The paper reviewed here showed, by numerically integrating the Langevin equation related to this process, that the efficiency of the energy transformation in a forced ratchet system can actually be optimised and that it is facilitated by thermal fluctuations, as Magnasco claimed.

2 The model

The Brownian dynamics of the overdamped particle, moving under the influence of an asymmetric potential $V_0(x)$ and subject to an external force field $F(t)$ at temperature T, is described by the following Langevin equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial}{\partial x}\left[V_0(x) + V_L(x)\right] + F(t) + \sqrt{2k_BT}\xi(t) \tag{1}$$

where $\xi(t)$ is a randomly fluctuating Gaussian white noise with zero mean and with autocorrelation function $\langle\xi(t)\xi(s)\rangle = \delta(t-s)$. $V_L(x)$ is a potential against which the work is done and $\partial/\partial x V_L = \lambda$ is the load force. The damping coefficient γ is absorbed in the time scale and temporal symmetry is applied.

A piece-wise linear but asymmetric ratchet potential, $V_0(x)$, of periodicity $L = 1$ is considered

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

Throughout the work, the value $a = 0.8$ and $Q = 1.$ is fixed. The periodic external driving force $F(t)$ has a square waveform

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

with a period τ 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.

A quantity of central interest is the time-averaged current J, or particles in the stationary state given by the relation

$$\langle \dot{x}(t) \rangle_{\mathrm{st}} = -\lambda + \frac{1}{\tau} \lim_{\tau \to \infty} \int_t^{t+\tau} \left\langle -\frac{\partial}{\partial s} V(s) + F(s) \right\rangle \mathrm{d}s = JL \tag{4}$$

where $V(x) = V_0(x) + V_L(x)$.

The efficiency is computed following the method of stochastic energetics. As usual, the efficiency η is defined as the ratio of useful work W done by the system pumping particles against the load force λ to the input of energy E_i from the external fluctuations

$$\eta = \frac{W}{E_i} \tag{5}$$

where

$$W = \frac{1}{\tau} \int_{x(n\tau)}^{x((n+1)\tau)} \mathrm{d}V[x(t)] = \lambda J \tag{6}$$

and

$$E_i = \frac{1}{\tau} \int_{x(n\tau)}^{x((n+1)\tau)} F(t) \mathrm{d}x(t) \simeq \frac{1}{\tau} \sum_{i=1}^{\tau/h} \cdot F(i \cdot h) \cdot \Delta x(i \cdot h) \tag{7}$$

where the last expression stands for the numerical approximation, being h the integration time step.

In order to obtain the results presented below, the Langevin equation, Eq. (1), has been integrated by means of the Milstein method using an integration time step of $h = 10^{-3}$ and averaging over 10^3 trajectories, eahc trajectory evolving over 50 periods ($t = 50\tau$).

The program used to retrieve all the results shown next can be found in https://github.com/agimenezromero/Forced-ratchet-model. It has been programmed in Julia and run in a MSI Intel Core i7-9750H CPU 2.60 GHz × 12 with 16 GB of RAM. The most demanding calculation, which involved the computation of the averaged Langevin equation several times, took 4 h. For the other calculations the elapsed time was between 5 min and 10 min.

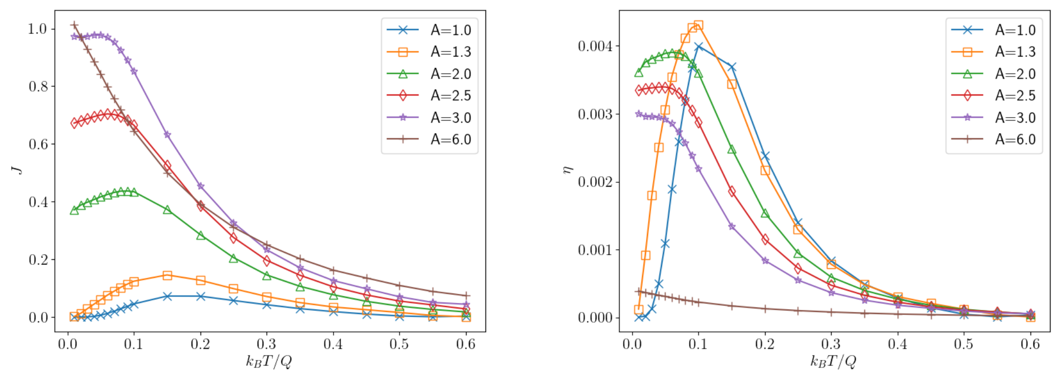
3 Results

First, the current ant efficiency have been computed as a function of the ratio $k_B T/Q$ (reduced temperature units) for the case where a zero mean external driving force is applied, so $\tau_1 = \tau/2$. The time period has been fixed to $\tau = 6$ and several values of the amplitude A have been considered. The load term has been set to $\lambda = 0.01$ for the whole work. In order to clarify the value of the parameters used, Table 1 summarises the values of the parameters that are kept constant in the whole study. The other parameters that will vary along the work will be mentioned in the text.

Table 1: Fixed parameters for all the simulations

L	λ	a	Q	h	t_f	Averages
1	0.01	0.8	1	10^{-3}	50τ	10^3

Fig. 1 show the current and the efficiency as a function of temperature (in reduced units) for $A \in [1, 1.3, 2, 2.5, 3, 6]$.



(a) J *vs* $k_B T/Q$

(b) η *vs* $k_B T/Q$

Figure 1: Current and efficiency as a function of $k_B T/Q$ for several values of A.

In Fig. 1(a) we can identify three different regimes

1. $A < Q/a + \lambda = 1.26$
2. $Q/a + \lambda < A < Q/(1-a) - \lambda = 4.99$
3. $A > Q/(1-a) - \lambda = 4.99$

The first two regimes correspond to low and moderate forcing and we can observe how the increase on temperature produces an increase and posterior decrease of the current. Thus, there is a finite temperature region where the current is optimised showing a clear maximum. In the third regime, for high amplitudes of the forcing, the current decreases monotonically as a function of the temperature, as the ratchet effect becomes unimportant in this regime. In Fig. 1(b) we see a similar behaviour, for low amplitudes of the forcing the efficiency attains a maximum at a finite temperature but as the amplitude increases this effect starts to disappear. At a very high amplitudes of the forcing the efficiency is too small and decreases monotonically. So, basically, it has been found already that the efficiency can be optimised at finite temperatures for low amplitude values of the driving force, proving the claim by Magnasco to be correct.

In order to understand the discrepancy with KHT we briefly present the arguments they followed. From the Langevin equation Eq. (1) the associated Fokker-Planck equation can be written in the form of a conservation law for the probability density $P(x,t), \partial_t P(x,t) + \partial_x j(x,t) = 0$ with a probability current obeying $j(x,t) = \left(f(x) + F(t) - k_B T \frac{\partial}{\partial x}\right) P(x,t)$. Assuming the solution for the probability density to be periodic in time and space the current can be solved for a **constant** driving force. Assuming that $F(t)$ varies slowly enough compared to any frequency in the problem, and for an external square waveform force of amplitude A it turns out that the average current can be written as

$$J = \frac{1}{2}\left[J(A) + J(-A)\right] \tag{8}$$

and the efficiency

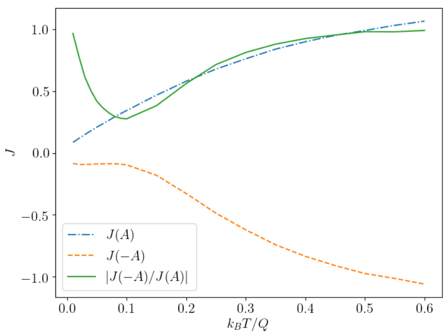
$$\eta = \frac{\lambda\left[J(A) + J(-A)\right]}{A\left[J(A) - J(-A)\right]} \tag{9}$$

that considering $J(-A) < 0$ turns into

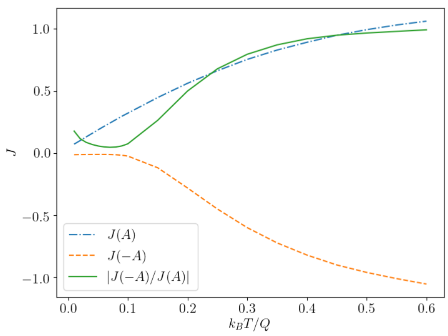
$$\eta = \frac{\lambda}{A}\left(\frac{1 - |J(-A)/J(A)|}{1 + |J(-A)/J(A)|}\right) \tag{10}$$

Eq. (10) that the efficiency depends exclusively on the ratio $|J(-A)/J(A)|$. If this ratio is monotonically increasing then η should be monotonically decreasing. KHT found exactly that the ratio $|J(-A)/J(A)|$ was a monotonically increasing function of the temperature causing the efficiency to be a monotonically decreasing function of temperature. Thus, their conclusion was that the efficiency could not be maximised for finite temperature values.

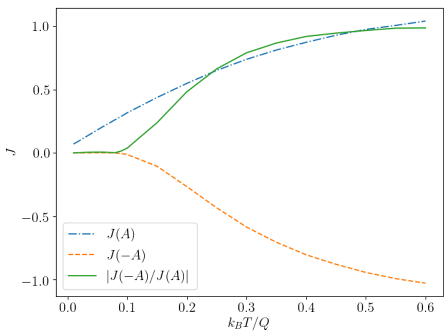
In the present work, the fluxes are analysed for different values of the period ($\tau = 6$, 50 and ∞) and a square waveform force field of amplitude $A = 1.3$. The case of $\tau = \infty$ basically represents a constant force of magnitude A.



(a) $\tau = 6$



(b) $\tau = 50$



(c) $\tau = \infty$

Figure 2: Plot of the currents for a field F(t) of a square waveform with amplitude $A = 1.3$ at different periods.

As can be observed in Fig. 2 as we increase the period of the force the ratio $|J(-A)/J(A)|$ approaches the theoretical limiting value of λ/A, matching it perfectly for $\tau = \infty$. Moreover, the minimum displayed in the case $\tau = 6$ is in the same temperature point that the maximum of the efficiency in Fig. 1(b), as we should expect.

For a further study of the influence of the period the efficiency for the case $\tau = 50$ has been computed for different amplitude values $A \in [1, 1.3, 2, 2.5, 3, 6]$.

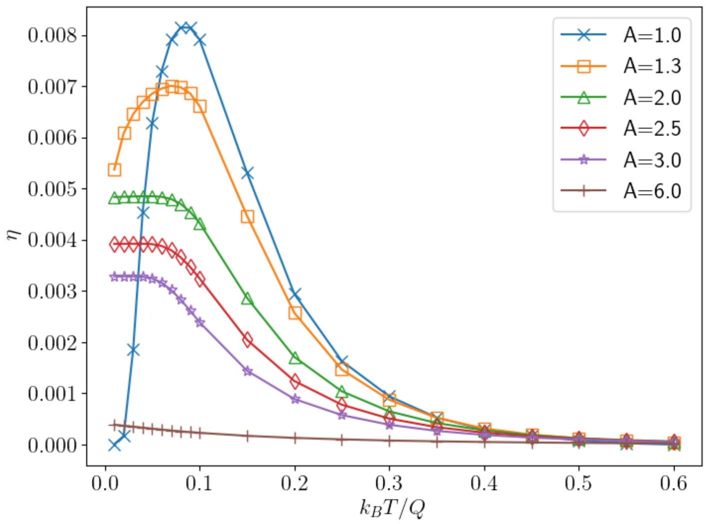


Figure 3: Efficiency as function of reduced temperature for $\tau = 50$

Comparing Fig. 3 with Fig. 1(b) we note that the curves for $A = 2$ and $A = 2.5$ which where giving clear optimal values in the case $\tau = 6$, now are monotonically decreasing with the temperature as found by KHT. However, for smaller values of A the peaks in the efficiency curve still exist and would follow the theoretical result only for much longer periods.
For increasing amplitude of the driving force A, the results obtained by KHT are qualitatively reproduced at finite τ values, and the ratio $|J(-A)/J(A)|$ is monotonically increasing. As an example, the results for $A = 3$ and $\tau = 6$ are plotted in Fig. 4.

Then, the results conclude that for sufficiently small values of the amplitude and period of the force, the efficiency of the forced ratchet can be optimised. Then, the presence of thermal fluctuations are important to improve the efficiency of energy transformation at low amplitudes of the forcing and the analytical result is valid only in the limiting case of $\tau \to \infty$.

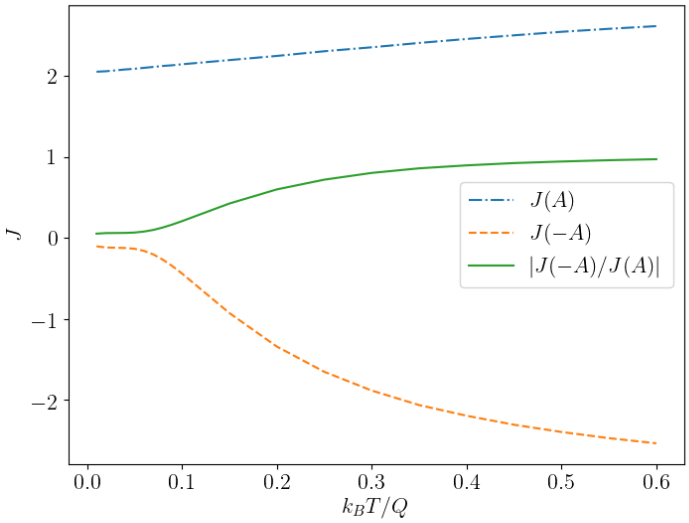
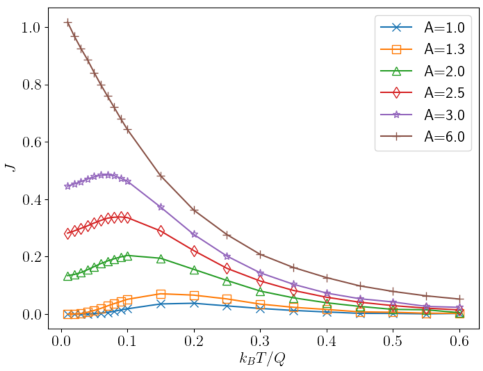
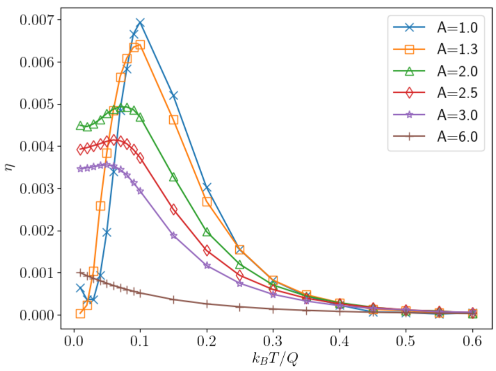


Figure 4: Same as Fig. 2 for $\tau = 6$ and $A = 3$.

We have also performed numerical simulations for a sinusoidal driving force of the form $F(t) = A\sin(\omega t)$. The frequency has been chosen to be $\omega = \pi/3$ as it corresponds to $\tau = 6$. The results plotted in Fig. 5 show the same qualitative behaviour than the square waveform force. Again, the efficiency can be optimised at finite temperature.



(a) J *vs* k_BT/Q

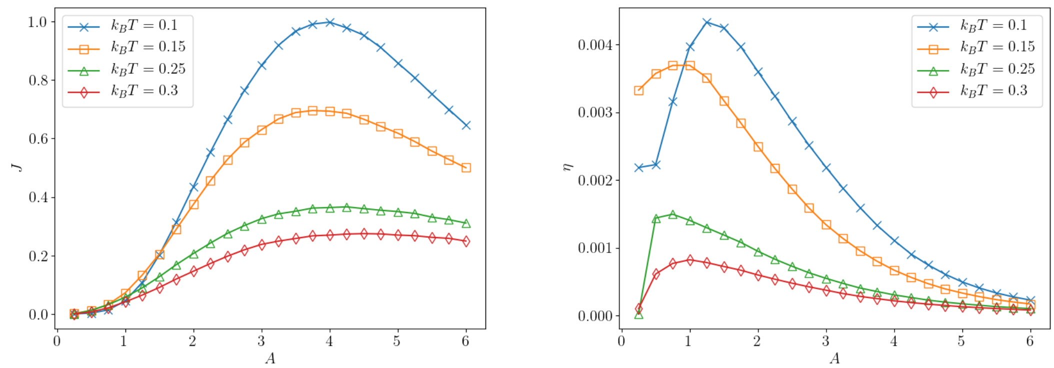


(b) η *vs* k_BT/Q

Figure 5: Current and efficiency as a function of k_BT/Q for $F = A\sin\omega t$ and several values of A.

For the square wave forcing as well as for the sinusoidal one, observe that the temperature associated with the maximum current J does not correspond with the one at which η is maximum. From this it can be concluded that the conditions for obtaining optimum current and efficiency are different as previously noted in other ratchet systems [1].

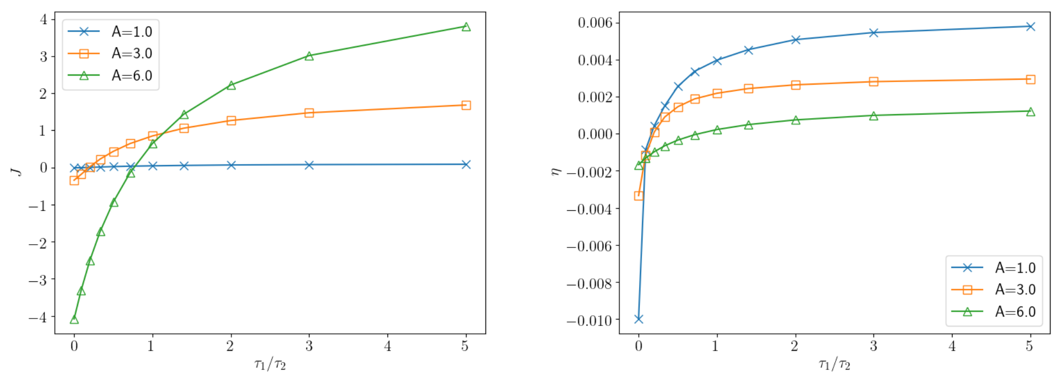
Then, we have studied the behaviour of the current and efficiency as a function of the amplitude A of an external driving force of a square waveform of periodicity $\tau = 6$. The results are shown in Fig. 6. It is clear that both the current and efficiency can be maximised with respect to the amplitude A. Smaller amplitudes are always preferred for having better efficiency and, as the amplitude goes to higher values, the ratchet becomes almost inefficient.



(a) J *vs* A (b) η *vs* A

Figure 6: Current and efficiency as a function of A for some values of k_BT/Q.

Finally, as all the calculations up to here were done keeping $t_1 = \tau/2$ constant, it is interesting to study how the current and efficiency varies with the time periods τ_1 and $\tau_2 \equiv \tau - \tau_1$ over which the system experiences a positive and a negative force, respectively. Fig. 7 shows current and efficiency as functions of the ratio between the time periods for several values of the driving force amplitude A.



(a) J *vs* τ_1/τ_2 (b) η *vs* τ_1/τ_2

Figure 7: Current and efficiency as a function of τ_1/τ_2 for some values of A.

The efficiency increases with the ratio in the same way the current does, and then attains a limiting value. The efficiency cannot be optimised with this ratio as in other previously studied different cases, as for instance the thermal ratchet pumps where it is maximised for ratios smaller than the unity.

4 Conclusions

In this work, the paper [1] by K. Sumithra and T.Sintes has been fully and successfully reproduced and reviewed, giving further support for their results claiming that efficiency in forced ratchets can be optimised due to thermal fluctuations.
As a summary, Langevin equation simulations have been done to investigate the energetics of an overdamped forced ratchet. In contradiction with the previous findings of KHT, the results reported here for a driving force of a square wave type and finite period τ, show that the efficiency of energy transformation can be optimised at finite temperatures in a spatially homogeneous system. This proves the claim made by Magnasco that there is a region of the operating regime where the efficiency can be optimised at finite temperatures.

References

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