Efficiency of Brownian motors

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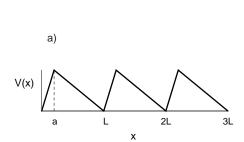
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Abstract. – The efficiency of different types of Brownian motors is calculated analytically and numerically. We find that motors based on flashing ratchets present a low efficiency and an unavoidable entropy production. On the other hand, a certain class of motors based on adiabatically changing potentials, named *reversible ratchets*, exhibit a higher efficiency and the entropy production can be arbitrarily reduced.

In the last years there has been an increasing interest in the so-called "ratchets" or Brownian motors [1-7]. These systems consist of Brownian particles moving in asymmetric potentials, such as the one depicted in fig. 1a), and subject to a source of non-equilibrium, like external fluctuations or temperature gradients. As a consequence of these two ingredients —asymmetric potentials and non-equilibrium—, a flow of particles can be induced.

Although these systems are sometimes called "Brownian or molecular motors", most of them do not convert heat into work. The reason is that the flow of particles is induced in a potential which is flat on average. Therefore, the Brownian particles do not gain energy in a systematic way. Feynman in his *Lectures* [8] already understood that, in order to have an engine out of a ratchet, it is necessary to use its systematic motion to store potential energy. This can be achieved if the ratchet lifts a load. In this way, Feynman estimated the efficiency of the ratchet as a thermal engine, although he followed assumptions which have been revealed to contain some inconsistencies [9]. For ratchets consisting of Brownian particles in asymmetric potentials, the load is equivalent to an external force opposite to the induced flow of particles. If the force is weak enough, particles still move against the force and their potential energy increases monotonically [7,10].

Recently, Sekimoto [10] has defined efficiency for a wide class of ratchets. Sekimoto studied a Brownian particle at a given temperature in a periodic potential which depends on the position x of the particle and on some parameter y. If this parameter y is modified, either deterministically or at random, by an external agent, then the increment of the internal energy of the system can be split into two contributions: dissipation, i.e. the heat transfer between the system and the thermal bath, and input energy, i.e. the energy transfer between the system and the external agent. As mentioned above, in the case of a ratchet with a weak external force (a load) opposite to the flow of particles, the average potential energy of the system increases monotonically. Then efficiency can be defined as the ratio between the potential energy gain and the input energy. This is the approach that we will follow in this letter.



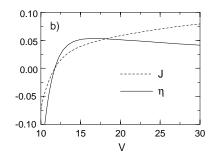


Fig. 1. – a) Asymmetric sawtooth potential of the ratchets presented in refs. [1-6]. In this letter we consider two types of ratchets: i) one where the potential is randomly switched on and off; and ii) one where the potential is deterministically modulated. b) Efficiency and current of the ratchet where the potential drawn in a) is randomly switched on and off (case i), as a function of the maximum height V of the potential. The reaction rates are $\omega_A = 1.08$ and $\omega_B = 81.8$, a = 1/11, and the external force is F = 4.145.

Jülicher et al. [7] have also discussed the efficiency of molecular motors from a different point of view. They consider ratchets where the source of non-equilibrium is a reaction occurring at a rate r, due to a chemical-potential difference $\Delta\mu$. Once again, a weak external force opposite to the flow of particles is included. The system becomes a chemical motor which can convert chemical energy into mechanical energy or vice versa and both a mechanical and a chemical efficiency can be defined. Finally, Sokolov and Blumen [11] have calculated the efficiency of a deterministically flashing ratchet in contact with two thermal baths at different temperatures. A general conclusion of these works is that motors based on ratchets are intrinsically irreversible, even in the quasi-static limit [7,9-11].

On the other hand, a class of deterministically driven ratchets where the entropy production vanishes in the quasistatic limit has been recently introduced [12]. We call them *reversible ratchets*, since, as we have shown in ref. [12], they can induce transport of particles in a reversible way, *i.e.* with zero entropy production, and without any energy consumption.

However, a load or external force was not considered in [12]. Consequently, motors based on reversible ratchets and their efficiency were not discussed in that paper. This is accomplished in this letter. Moreover, here we explore the differences, regarding efficiency, among randomly flashing ratchets and both reversible and irreversible deterministically driven ratchets.

Randomly flashing ratchets. — Consider two species of Brownian particles, say A and B, moving in the interval [0, L] with periodic boundary conditions. Let us assume that a potential $V_A(x)$ acts on A particles, whereas a different potential, $V_B(x)$, acts on B particles. Besides, there is a continuous exchange of particles, $A \rightleftharpoons B$, which accounts for non-equilibrium fluctuations. From now on, and following ref. [10], we will refer to this reaction as the external agent. It is easy to check that this system with two species of particles is equivalent to that of a single Brownian particle in a randomly switching potential [4].

In ref. [4], it was proved that a flow towards a given direction, say, to the right, occurs for some asymmetric potentials V_A and V_B . If we add a load or force F opposite to the flow, the evolution equation for the probability densities of particles A and B reads

$$\partial_t \rho_A(x,t) = -\partial_x \mathcal{J}_A \rho_A(x,t) - \omega_A \rho_A(x,t) + \omega_B \rho_B(x,t) ,$$

$$\partial_t \rho_B(x,t) = -\partial_x \mathcal{J}_B \rho_B(x,t) + \omega_A \rho_A(x,t) - \omega_B \rho_B(x,t) ,$$
(1)

where $\mathcal{J}_i = -V_i'(x) - F - \partial_x$ is the *current operator*, the prime indicates derivative with respect

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to x, and ω_A and ω_B are the rates of the reactions $A \to B$ and $B \to A$, respectively. We have taken units of energy, length and time such that the temperature is $k_BT = 1$, the length of the interval is L = 1, and the diffusion coefficient is D = 1.

The flow of particles in the stationary regime is $J = \mathcal{J}_A \rho_A^{\rm st}(x) + \mathcal{J}_B \rho_B^{\rm st}(x)$, where $\rho_{A,B}^{\rm st}(x)$ are the stationary solutions of eq. (1). The flow J is a decreasing function of the external force F and becomes negative if F is stronger than a *stopping force*, $F_{\rm stop}$. Therefore, if $0 < F < F_{\rm stop}$, particles move against the force and, consequently, gain potential energy in a systematic way. The potential energy gain or *output energy* per unit of time is

$$E_{\text{out}} = JF, \qquad (2)$$

which vanishes both for F = 0 and $F = F_{\text{stop}}$.

On the other side, the reaction $A \rightleftharpoons B$ does not conserve energy since $V_A(x) \neq V_B(x)$. Therefore, in every reaction $A \to B$, occurring at a point x, $V_B(x) - V_A(x)$ is the energy transfer from the external agent to the system. Similarly, $V_A(x) - V_B(x)$ is the energy transfer in every reaction $B \to A$ occurring at x. In the stationary regime, the average number of such reactions per unit of time is, respectively, $\omega_A \rho_A^{\rm st}(x)$ and $\omega_B \rho_B^{\rm st}(x)$. Therefore, the *input energy* per unit of time is [10]

$$E_{\rm in} = \int_0^1 \mathrm{d}x \left[V_B(x) - V_A(x) \right] \left[\omega_A \rho_A^{\rm st}(x) - \omega_B \rho_B^{\rm st}(x) \right] . \tag{3}$$

Finally, the efficiency can be defined as

$$\eta = \frac{E_{\text{out}}}{E_{\text{in}}} \,. \tag{4}$$

The efficiency η can be calculated analytically for the system given by eq. (1) with piecewise potentials. We have performed an exhaustive study for the particular setting $V_B(x) = 0$ and $V_A(x)$ equal to the potential depicted in fig. 1a):

$$V_A(x) = \begin{cases} Vx/a, & \text{if } x \le a, \\ V(1-x)/(1-a), & \text{if } x \ge a \end{cases}$$
 (5)

with a=1/11. For a symmetric reaction, $\omega=\omega_A=\omega_B$, the maximum efficiency is $\eta_{\rm max}=3.29\%$, which is reached for V=22, F=3, and $\omega=63$. The efficiency slightly increases for different reaction rates. In this case, $\eta_{\rm max}=5.315\%$, which is reached for V=16.7, F=4.145, $\omega_A=1.08$, and $\omega_B=81.8$. Observe that, with these values for ω_A and ω_B , the particle remains much longer within the potential $V_A(x)$ than within $V_B(x)$.

We have plotted in fig. 1b) the efficiency and the flow of particles as a function of V, setting the rest of parameters equal to the optimal values described above. Two are the messages from this figure. Firstly, the maximization of the efficiency is a new criterion to define optimal Brownian motors. Notice that this criterion is not as trivial as that of maximizing the flow in some situations as, for instance, when V runs from zero to infinity.

Secondly, the randomly flashing ratchet under study has a rather low efficiency. Let us compare the efficiency that we have obtained with the upper bound given by the Second Law of Thermodynamics. To do that, we have to evaluate the changes of entropy in each part of the model: the thermal bath, ΔS_{bath} , the Brownian particles, ΔS_{sys} , and the external agent, ΔS_{ext} . As we have mentioned before, the heat dissipation to the thermal bath per unit of time is $E_{\text{in}} - E_{\text{out}}$. Consequently, the increase of entropy of the thermal bath, per unit of time, is $\Delta S_{\text{bath}} = k_{\text{B}}(E_{\text{in}} - E_{\text{out}})$, since $k_{\text{B}}T = 1$. On the other hand, in the stationary

regime the entropy of the system is constant, $\Delta S_{\rm sys} = 0$. It is not an easy task to calculate the change of entropy of the external agent, since we have not specified a physical model for it. Nevertheless, we can give here some plausibility arguments to show that the external agent can be interpreted as a second thermal bath at infinite temperature (see also [11] for an interpretation of the deterministically flashing ratchet as a thermal engine in contact with a bath at infinite temperature). To see this, assume that the external agent is at temperature $T_{\rm ext}$ and induces the reactions $A \to B$ and $B \to A$ obeying detailed balance with respect to $T_{\rm ext}$. Then $\omega_A = \omega_B \exp\left[-(V_B(x) - V_A(x))/(k_B T_{\rm ext})\right]$, where the reaction rates depend on the position x. If $T_{\rm ext} = T$, the system reaches thermal and chemical equilibrium and no flow is induced, whereas if $T_{\rm ext}$ is infinite we recover our model with $\omega_A = \omega_B$. Thus, for the flashing ratchet, the entropy of the external agent remains constant: $\Delta S_{\rm ext} = -E_{\rm in}/T_{\rm ext} = 0$. Finally, the net entropy production per unit of time is $\Delta S = \Delta S_{\rm bath} + \Delta S_{\rm sys} + \Delta S_{\rm ext} = k_{\rm B}(E_{\rm in} - E_{\rm out})$. If this entropy production vanished, *i.e.* if the system worked in a reversible way, it would reach a 100% efficiency. However, the efficiency is below 10% and we can conclude that the motor based on the randomly flashing ratchet is very inefficient.

One could think that the efficiency would increase in situations where the system is close to equilibrium, such as $\omega = \omega_A = \omega_B \to 0$ and/or $V_A - V_B \to 0$. However, a perturbative analysis of eq. (1) shows that $\eta \to 0$ in both limits. In the first case, $\omega \to 0$, from eq. (1) one can easily find that J is of order ω , so is F_{stop} . Therefore, E_{out} , in the interval $0 < F < F_{\text{stop}}$, is of order ω^2 , whereas one can prove that E_{in} is of order ω , giving a zero efficiency in this limit. In the second case, $\Delta V(x) \equiv V_A(x) - V_B(x) \to 0$, the input energy E_{in} is of order ΔV^2 . However, surprisingly enough, J is of order ΔV^2 and so is F_{stop} . Hence, E_{out} is of order ΔV^4 and the efficiency vanishes. Notice that this argument is also valid when $V_A(x) - V_B(x)$ tends to an arbitrary constant, since this constant neither appears in the evolution equation (1) nor contributes to the input energy given by (3). We conclude that the flashing motor is intrinsically irreversible, as has been pointed out for related models in refs. [7,9-11].

Deterministically driven ratchets. — As a different strategy to reduce the entropy production, we consider Brownian particles in a potential which changes deterministically in time. If the potential changes slowly, the system evolves close to equilibrium and the entropy production is low. From now on, we will focus our attention on Brownian particles in a spatially periodic potential $V(x; \mathbf{R}(t))$ depending on a set of parameters collected in a vector \mathbf{R} [12]. The parameters are changed periodically in time with period T, i.e. $\mathbf{R}(0) = \mathbf{R}(T)$.

As in ref. [10], we have to modify our definition of efficiency. Firstly, we deal with energy transfer per cycle [0, T] instead of per unit of time. Secondly, the input energy or work done to the system in a cycle, as a consequence of the change of the parameters $\mathbf{R}(t)$, is

$$E_{\rm in} = \int_0^T dt \int_0^1 dx \, \frac{\partial V(x; \mathbf{R}(t))}{\partial t} \rho(x, t) \,. \tag{6}$$

The probability density $\rho(x,t)$ verifies the Smoluchowski equation

$$\partial_t \rho(x,t) = -\partial_x \mathcal{J}_{\mathbf{R}(t)} \rho(x,t) \,, \tag{7}$$

where $\mathcal{J}_{\mathbf{R}} = -V'(x; \mathbf{R}) - F - \partial_x$ is the current operator corresponding to the potential $V(x; \mathbf{R})$. As before, the output energy is the current times the force F, but now the current is not stationary and we have to integrate along the process:

$$E_{\text{out}} = \int_0^T dt \ F \mathcal{J}_{\mathbf{R}(t)} \rho(x, t) = F \phi, \qquad (8)$$

where ϕ is the integrated flow along the process.

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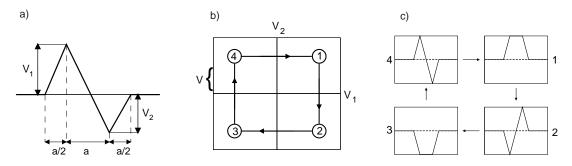


Fig. 2. – Graphical representation of the reversible ratchet described in the text: the potential in a) depends on two parameters, V_1 and V_2 , which are the height/depth of two barriers/wells and they change along the path depicted in b), V being the maximum height/depth of the barriers/wells. In c), the shape of the potential at the four labelled points is shown.

With the above expressions, the efficiency of the system, $\eta = E_{\text{out}}/E_{\text{in}}$, can be found analytically for T large and weak external force, where η is expected to be high. The integrated flow ϕ and the input energy E_{in} can be obtained by solving eq. (7) perturbatively up to first order of $\dot{\mathbf{R}}(t)$ and inserting the solution in eqs. (6) and (8). This procedure is similar to that carried out in ref. [12] for the particular case F = 0. For the integrated flow one finds

$$\phi = \phi_0 - \bar{\mu}FT \,, \tag{9}$$

where $\bar{\mu}$ is the average mobility of the system:

$$\bar{\mu} = \frac{1}{T} \int_0^T \frac{\mathrm{d}t}{Z_+(\mathbf{R}(t))Z_-(\mathbf{R}(t))} \tag{10}$$

and ϕ_0 is the integrated flow for F=0 [12]:

$$\phi_0 = \oint d\mathbf{R} \cdot \int_0^1 dx \int_0^x dx' \rho_+(x; \mathbf{R}) \nabla_{\mathbf{R}} \rho_-(x'; \mathbf{R}) , \qquad (11)$$

with

$$\rho_{\pm}(x;\mathbf{R}) \equiv \frac{e^{\pm V(x;\mathbf{R})}}{Z_{\pm}(\mathbf{R})}; \quad Z_{\pm}(\mathbf{R}) \equiv \int_0^1 \mathrm{d}x \ e^{\pm V(x;\mathbf{R})} \,.$$

In eq. (11) the contour integral runs over the closed path $\{\mathbf{R}(t):t\in[0,T]\}$ in the space of parameters of the potential. The term proportional to T in eq. (9) arises because the force F induces a non-zero current which is present along the whole process. As a consequence, the stopping force is $F_{\text{stop}} = \phi_0/\bar{\mu}T$. Therefore, in order to design a motor in the adiabatic limit, it is necessary to take simultaneously the limits $T \to \infty$ and $F \to 0$, with $\alpha \equiv FT$ finite.

Observe that the above expressions are useless if $\phi_0 = 0$. In ref. [12], we have called reversible ratchets those systems exhibiting transport in the adiabatic limit, i.e. with $\phi_0 \neq 0$. This is satisfied by potentials $V(x; \mathbf{R})$ depending on two or more parameters such as the one depicted in fig. 2, which is a modification of the example discussed in [12]. From now on, we restrict our analytical calculations to reversible ratchets, although we also present numerical results for an irreversible ratchet below.

The input energy given by eq. (6), up to first order on F and 1/T, is

$$E_{\rm in} = \phi_0 F + b/T \tag{12}$$

6

8

4

α

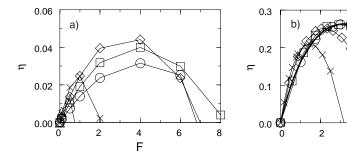


Fig. 3. – a) Irreversible ratchet: numerical results for the efficiency of the ratchet consisting of the potential in fig. 1 a) modulated by $z(t) = \cos^2(\pi t/T)$ as a function of the external force F and for different values of the period T: T=0.00125 (o), 0.025 (\Box), 0.05 (o), 0.25 (×), and 0.5 (a). b) Reversible ratchet: numerical and analytical results for the efficiency of the ratchet described in fig. 2 for V=5 a=0.2 as a function of $\alpha \equiv FT$ and for different values of the period T: T=1 (×), T=10, T=11 (×), T=11 (×),

with

$$b = -\int_0^T dt \ Z_{-}(\mathbf{R}(t)) Z_{+}(\mathbf{R}(t)) \left\{ \left[\int_0^1 dx \int_0^x dx' \ \rho_{+}(x; \mathbf{R}(t)) \left[\partial_t \rho_{-}(x'; \mathbf{R}(t)) \right] \right]^2 + \int_0^1 dx \int_0^x dx' \int_0^{x'} dx'' \left[\partial_t \rho_{-}(x; \mathbf{R}(t)) \right] \rho_{+}(x'; \mathbf{R}(t)) \left[\partial_t \rho_{-}(x''; \mathbf{R}(t)) \right] \right\},$$
(13)

which is a positive quantity. Combining the above expressions, one finds for the efficiency

$$\eta = \frac{F\phi}{E_{\rm in}} = \frac{F(\phi_0 - \bar{\mu}FT)}{\phi_0 F + b/T} = \frac{\phi_0 \alpha - \bar{\mu}\alpha^2}{\phi_0 \alpha + b},\tag{14}$$

where $\alpha \equiv FT$. This expression is exact in the limit $T \to \infty$, $F \to 0$. Notice that, even for large T, the irreversible contribution, b/T, to $E_{\rm in}$ is of the same order as $\phi_0 F$.

In a given system, *i.e.* for a set of parameters ϕ_0 , $\bar{\mu}$ and b, the maximum efficiency is reached for $\alpha = (b/\phi_0)[\sqrt{1+\phi_0^2/(\bar{\mu}b)}-1]$ and its value is given by

$$\eta_{\text{max}} = 1 - 2\left[\sqrt{z(1+z)} - z\right] \tag{15}$$

with $z = b\bar{\mu}/\phi_0^2$. Equation (15) clearly shows how the term b in the denominator of eq. (14) prevents the system from reaching an efficiency equal to one. Fortunately, as we will see in a particular example below, using strong potentials one can get arbitrarily close to 100% efficiency.

To check the validity of the above theory and to stress the differences between reversible and irreversible ratchets, we have studied in detail one example of each class.

As an example of irreversible ratchet, consider the modulation of the potential in fig. 1a), i.e. $V(x;t) = \cos^2(\pi t/T)V(x)$ with V(x) given by eq. (5). In this case, ϕ_0 is zero and the above theory cannot be applied. We have numerically integrated the Smoluchowski equation, eq. (7), using an implicit scheme with $\Delta t = 10^{-5}$, $\Delta x = 0.002$, 0.005, and the Richardson extrapolation method to correct inaccuracies coming from the finite Δx . The efficiency has been obtained using eqs. (4), (6), (8) and the results, as a function of F and for different values

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of T, are plotted in fig. 3a). The efficiency is maximum for T around 0.5 and it goes to zero as T increases. The maximum efficiency found by numerical integration is of the same order of magnitude as the one found for the randomly flashing ratchet. Notice, however, that we cannot explore the whole space of parameters with numerical experiments.

On the other hand, let us consider the reversible ratchet represented in fig. 2. Here the potential depends on two parameters, V_1 and V_2 , which are the heights/depths of two triangular barriers/wells of width a. We modify at a constant velocity the parameters V_1 and V_2 along the path depicted in fig. 2b). Now ϕ_0 does not vanish and the above theory gives us the efficiency in the limit $T \to \infty$ and $F \to 0$. For instance, for V = 5 and a = 0.2, we obtain $\phi_0 = 0.825$, $\bar{\mu} = 0.094$ and b = 3.74. The efficiency given by eq. (14) is plotted in fig. 3b) and is compared with a numerical integration of the Smoluchowski equation for different values of T. Notice the differences with the irreversible ratchet. Here the efficiency is an increasing function of T. The maximum efficiency, for the parameters corresponding to fig. 3b), is 26% which is almost reached for T = 40. The efficiency of this ratchet can be arbitrarily close to 100% if V is increased. The reason is that the average mobility decreases exponentially with V, but the coefficient b and the integrated flow ϕ_0 remain finite. For instance, for V = 20 and a = 0.4, $\phi_0 = 0.999988$, b = 6.89 and $\bar{\mu} < 10^{-7}$, giving a maximum efficiency of 99.85%.

Finally, it should be stressed that our engine works by means of a genuine ratchet mechanism, namely, the rectification of thermal fluctuations. As a matter of fact, the engine does not work at zero temperature, since the crossing through x=0, occurring essentially between steps 4 and 2, is due to thermal fluctuations.

To summarize, we have calculated the efficiency of a randomly flashing ratchet with an asymmetric sawtooth potential. In order to find more efficient Brownian motors, we have also calculated the efficiency of deterministically driven ratchets, finding that the efficiency of reversible ratchets is much higher than the efficiency of irreversible ratchets. It is remarkable that the class of reversible ratchets involves potentials depending on two or more parameters [12] and they differ from the models considered to date in the literature. Here we have shown that this new and non-trivial class of ratchets is a real breakthrough regarding efficiency.

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