Optimal operation of feedback flashing ratchets

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Received 26 May 2008
Accepted 25 August 2008
Published 6 January 2009

Abstract. Feedback flashing ratchets are thermal rectifiers that use information on the state of the system to operate the switching on and off of a periodic potential. We discuss different strategies for this operation with the aim of maximizing the net flux of particles in the collective version of a flashing ratchet consisting of $N$ overdamped Brownian particles. We show the optimal protocols for the one-particle ratchet and for the collective ratchet with an infinite number of particles. Finally we comment on the unsolved problem of the optimal strategy for any other number of particles.

Keywords: stochastic particle dynamics (theory), molecular motors (theory)
1. Introduction

Brownian motors or ratchets are rectifiers of thermal fluctuations that induce direct transport without an a priori bias [1]. The breaking of thermal equilibrium and of certain time–space symmetries are necessary conditions to manage direct transport [2]–[4]. Ratchets are relevant from the theoretical point of view to study non-equilibrium processes, and from a practical point of view due to their applications in nanotechnology and biology [1, 5, 6]. A prototypical example of a ratchet system is the so-called flashing ratchet, which is based on switching on and off a periodic potential [7, 8]. The spatial asymmetry of the potential ensures a direct transport, but also a symmetric potential under an intrinsically asymmetric operation for the switching can achieve this task. Figure 1 illustrates the operation of a flashing ratchet.

Control strategies such as those obtained with a time-periodic or random switching are open-loop control policies, as they do not use any information about the particle distribution in the system to operate. Some studies deal with the optimal modulation in time of the ratchet potential to maximize the performance of these open-loop systems [9, 10]. These works use a variational approach to optimize the velocity induced by deterministic modulation in time of the potential.

On the other hand, it has been shown that a significant increase for the net flux in a flashing ratchet can be obtained if feedback on the state of the system is used by the protocol that switches on and off the ratchet potential [11] (i.e. taking into account the positions of the Brownian particles before the switching operation). This can improve the technological applications of ratchets. Experimental implementations of these feedback (=closed-loop control) flashing ratchets have been proposed [12]–[14], and the realization of such devices is currently underway [14, 15]. In addition, feedback ratchets have been suggested as a mechanism to explain the stepping motion of the two-headed kinesin [16] and are also present in other chemically driven molecular motors [17]–[19].

In this context, determining the optimal protocol for the operation of collective feedback ratchets is a relevant question that has only received partial answers. In the present work we review and compare some control strategies designed with the aim of
maximizing the net flux of particles. We show the optimal protocol for the one-particle flashing ratchet and for the limit case of an infinite number of particles. In section 2 we present the Langevin equations standing for the feedback ratchet. After that, we revise the instant maximization protocol (section 3), the threshold protocol (section 4) and the maximal net displacement protocol (section 5). We finally discuss the main unsolved questions related to the optimal operation of these systems (section 6).

2. Collective flashing ratchet

A collective flashing ratchet can be modelled by N Brownian particles at positions \( \{x_j(t)\} \) that satisfy the overdamped Langevin equations

\[
\gamma \dot{x}_i(t) = \alpha(\{x_j(t)\}, t) F(x_i(t)) + \xi_i(t); \quad i = 1, \ldots, N. 
\]

Here, \( F(x) = -V'(x) \), with \( V(x) \) the so-called ratchet potential, which is usually spatially periodic, \( V(x) = V(x + L) \), and has broken symmetry \( x \rightarrow -x \). In these equations \( \xi_i(t) \) stand for Gaussian white noises of zero mean and variance \( \langle \xi_i(t)\xi_j(t') \rangle = 2\gamma k_B T \delta_{ij} \delta(t-t') \), with \( \gamma \) the viscous friction coefficient. The function \( \alpha(t) \) implements the action of a controller that switches on the ratchet potential \( (\alpha = 1) \) or switches it off \( (\alpha = 0) \). Thanks to this switching, detailed balance symmetry is broken and the system can act as a Brownian motor. Note that, even for symmetric potentials \( V(x) = V(-x) \), there can be a ratchet effect provided the control policy induces the required asymmetry.

doi:10.1088/1742-5468/2009/01/P01031
A common ratchet potential is
\[ V(x) = V(x + L) = \frac{2V_0}{3\sqrt{3}} \left[ \sin \left( \frac{2\pi x}{L} \right) + \frac{1}{2} \sin \left( \frac{4\pi x}{L} \right) \right], \] (2)
which has height \( V_0 \) and asymmetry parameter \( a = 1/3 \) (with \( aL \) the distance between a minimum and the next maximum). This potential has been used in figure 1 to illustrate the flashing ratchet effect.

It is worthwhile to point out that there is no dependence of the average flux on the number of particles for open-loop control policies, as the Langevin equations are decoupled. However, for closed-loop ratchets the feedback strategy introduces a coupling between the particle dynamics, and the centre-of-mass velocity does depend on \( N \).

3. The instant maximization protocol

In the instant maximization of the velocity protocol [11] the control policy depends on the sign of the net force per particle at each instant of time. More specifically, the potential is switched on if the net force the particles would feel with the potential ‘on’:
\[ f(t) = \frac{1}{N} \sum_{i=1}^{N} F(x_i(t)), \] (3)
is positive, and the potential is switched off otherwise. Thus
\[ \alpha(t) = \Theta(f(t)), \] (4)
with \( \Theta \) the Heaviside function (\( \Theta(x) = 1 \) if \( x > 0 \), else \( \Theta(x) = 0 \)).

For a one-particle ratchet this protocol gives the maximum possible flux, i.e. it is the optimal protocol for \( N = 1 \). Let us call \( x \) the cyclic coordinate of the particle (modulo \( L \)). Then, the instant maximization protocol just consists of switching on the potential whenever the particle is in a region with a positive slope of the potential, \( x \in (aL, L) \), or switching off the potential whenever the particle is in a region with a negative slope, \( x \in (0, aL) \). Hence the system can be reinterpreted as a Brownian particle that freely diffuses in the flat regions \( (aL, L) \) and ‘slides down’ in the biased regions \( (0, aL) \). Now it is clear that the instant maximization protocol is the optimal strategy for the one-particle ratchet, as any change in the prescription \( \alpha(x(t)) \) would imply either changing the flat regions to uphill potential barriers or changing the downhill regions to plateaus. A similar argument allows us to prove the more general statement that the instant maximization protocol beats any general protocol \( \alpha(x(t), t) \), even with an explicit dependence on \( t \) and \( \alpha \) varying in the range \([0, 1]\) (pulsating ratchets). From the Langevin equation (1), with \( N = 1 \), the average steady state velocity is formally computed as
\[ \langle \dot{x} \rangle = \lim_{\tau \to \infty} \frac{1}{\gamma \tau} \int_0^\tau \alpha(x(t), t)F(x(t)) \, dt. \] (5)

On the other hand, the effective force including the action of the controller in the instant maximization operation is \( \Theta(F(x(t)))F(x(t)) \), so that at each instant of time \( t \) the inequality
\[ \alpha(x(t), t)F(x(t)) \leq \Theta(F(x(t)))F(x(t)) \] (6)
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Figure 2. Stationary centre-of-mass velocity as a function of the number of particles for the instant maximization protocol and for the threshold protocol with optimal thresholds for $N \to \infty$. The dashed line stands for the periodic switching protocol with optimal periods. Units: $L = 1$, $\gamma = 1$, $k_B T = 1$. We have used the ratchet potential (2) with potential height $V_0 = 5$. For this system the optimal thresholds for $N \to \infty$ are $u_{\text{on}} \simeq 0.6$ and $u_{\text{off}} \simeq -0.4$. The estimated optimal semiperiods for the on and off times of the periodic protocol are 0.06 and 0.05, respectively.

holds for any control $0 \leq \alpha(x(t), t) \leq 1$, as the maximum value for a positive (negative) force is obtained when the control parameter is $\alpha = 1$ ($\alpha = 0$). We finally combine inequality (6) and equation (5), which proves the optimality of the instant maximization protocol.

However, for a large number of particles the system dynamics gets trapped with the potential ‘on’ or ‘off’, as the fluctuations of the magnitude of $f(t)$—which trigger the switches—become smaller [11]. Therefore useless waiting times with the particle distribution near the equilibrium are wasted after the next switching. For a thousand particles the instant maximization protocol gives a lower flux than a simple periodic switching strategy that does not receives any feedback from the system. In the end, the flux goes to zero as $N$ increases; see figure 2.

4. The threshold protocol

The undesired trapping of the many-particle dynamics is settled in the threshold protocol [20, 21], in which the potential switchings are forced, provided the magnitude of the net force is below certain threshold values and the system is in an unproductive state near equilibrium.

Let us call $u_{\text{on}} \geq 0$ and $u_{\text{off}} \leq 0$ the threshold values that induce switchings off and on when the decaying long tails of $f(t)$ are still positive or negative, respectively. Then,
the threshold control is given by

\[
\alpha(t) = \begin{cases} 
1 & \text{if } f(t) \geq u_{\text{on}}, \\
1 & \text{if } u_{\text{off}} < f(t) < u_{\text{on}} \quad \text{and} \quad \dot{f}_{\text{exp}}(t) \geq 0, \\
0 & \text{if } u_{\text{off}} < f(t) < u_{\text{on}} \quad \text{and} \quad \dot{f}_{\text{exp}}(t) < 0, \\
0 & \text{if } f(t) \leq u_{\text{off}}.
\end{cases}
\]  

The condition over the sign of the derivative of the net force ensures that the switchings are only enforced when the system is really relaxing to equilibrium. This derivative is obtained by applying the Itô chain rule to the stochastic magnitude \( f(t) \) [20, 21]:

\[
\dot{f}_{\text{exp}}(t) = \frac{1}{\gamma N} \sum_i \alpha(t) F(x_i(t)) F'(x_i(t)) + \frac{k_B T}{\gamma N} \sum_i F''(x_i(t)).
\]

The instant maximization protocol—optimal for \( N = 1 \)—is recovered by taking zero threshold \( u_{\text{on}} = u_{\text{off}} = 0 \). On the other hand, for an adequate value of the thresholds, this new strategy gives the same flux as the optimal periodic, open-loop switching protocol for an infinite number of particles. Note that for \( N \to \infty \) no appreciable advantage over the optimal periodic switching can be obtained by using a feedback scheme, as only one degree of freedom is performed in the control (switching on and off). Therefore, the family of threshold protocols succeeds in getting the optimal control both for the one-particle case and for the infinite-particle case, yielding in between fluxes greater than or equal to open-loop protocols for all numbers of particles. In fact, the specific thresholds \( u_{\text{on}} \) and \( u_{\text{off}} \) that are optimal for \( N \to \infty \) also give a high value for the flux close to the value corresponding to the best thresholds for finite \( N \) [21]. Figure 2 shows the flux dependence with the number of particles for the instant maximization protocol and the threshold protocol with optimal thresholds for \( N \to \infty \). The flux is also compared with the \( N \)-independent value for the best open-loop, periodic switching protocol.

5. The maximal net displacement protocol

The previous feedback control strategies are based on the distribution of the forces \( \{F(x_i)\} \). But other choices are also possible. For instance, in the so-called maximal net displacement protocol [14] the control parameter depends on the particle distribution as follows:

\[
\alpha(t) = \Theta(d(t)); \quad d(t) = \sum_{i=1}^{N} (x_i(t) - x_0),
\]

where \( x_0 \) is the mean of a Gaussian distribution at equilibrium in the ratchet potential \( V(x) \). This new protocol was numerically found [14] to slightly beat the instant maximization protocol for collective ratchets of two and three particles and potential heights \( \gtrsim 30 k_B T \). However, it performs worse for other numbers of particles or smaller potential heights.
6. Discussion and open questions

The previous results provide some partial answers to the question of the optimal operation of feedback ratchets to maximize the flux. The appropriate introduction of feedback policies in collective flashing ratchets improves the performance of the system for a finite number of particles. In particular, the instant maximization protocol [11] is the optimal operation for the one-particle ratchet, as we have proven. However, this ‘greedy’ strategy is not optimal for the collective version of the ratchet. This kind of short-range maximization has also been reported not to be optimal in the so-called paradoxical games [22, 23]. On the other hand, in the limit of an infinite number of particles no advantage over open-loop strategies can be achieved by using any feedback in the system. Our results also show that the threshold protocol [20, 21] with proper threshold values is optimal for \( N = 1 \) (zero thresholds) and \( N \to \infty \), and it can give large values of the flux for intermediate numbers of particles. It is interesting to note that an exact optimization study in the framework of a discrete ratchet-like system revealed that the optimal protocol is indeed a kind of threshold operation [23].

Despite the advance that these partial answers represent, the fundamental problem— which is the optimal protocol for a collective feedback flashing ratchet—is still unsolved. A systematic study about the maximization of the flux in these systems using either the stochastic version of the Pontryagin maximum principle or the stochastic version of Bellman’s dynamic programming [24] is still lacking. On the other hand, we point out that adding another external perturbation to the feedback flashing ratchet can enlarge the flux of the system, as it happens, for instance, when a feedback flashing ratchet is rocked with proper amplitude and frequency [25]. We also point out that, to the best of our knowledge, there is still no study of the effects of inertia in feedback ratchets. These studies will also broaden the implications and applications of feedback ratchets.

Finding the optimal protocol of feedback ratchets would be an important theoretical task, as these systems are nothing other than Maxwell’s demons [26]; thus it would give a paradigmatic example to illustrate the maximum performance that can be attained by using a certain amount of information obeying thermodynamic restrictions. On the other hand, there is also an increasing interest in feedback flashing ratchets as nanotechnological devices (see [14] for a description of two set-ups capable of implementing a collective feedback flashing ratchet; one of these experiments has been very recently done [15]). In addition, the maximization of the instant velocity, which is optimal for \( N = 1 \) as we have proved, has allowed one to get an insight into the motion of a linear, two-headed, processive molecular motor [16]. A deep knowledge of the maximum flux that can be attained in feedback flashing ratchets could also help to get an insight into other biological systems, such as molecular motors operating in a collective way [27].

Acknowledgments

We acknowledge financial support from MCYT (Spain) through the Research Project FIS2006-05895, from the ESF Programme STOCHDYN, and from UCM and CM (Spain) through CCG07-UCM/ESP-2925.

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doi:10.1088/1742-5468/2009/01/P01031

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