The flashing ratchet: long time behavior and dynamical systems interpretation

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Abstract. The flashing ratchet is a model for certain types of molecular motors as well as a convenient model problem in the more general context of diffusion mediated transport. In this paper we show that it can be derived using a minimum energy dissipation principle for transport in a viscous environment. We then study the long time behavior of the flashing ratchet model. By entropy methods, we prove the existence of periodic solutions which are global attractors for the dynamics, with an exponential rate. Large time qualitative behaviour and especially mass accumulation are then investigated from a numerical point of view. For that purpose, we introduce a numerical method based on the minimum energy dissipation principle, which allows us to reduce the problem to a simple dynamical system.

Keywords. Linear parabolic equations – flashing ratchet – Brownian motors – molecular ratchets – mass transfer problem – Wasserstein distance – transfer function – Monge-Ampère equation – gradient flow – steepest descent – minimum energy dissipation principle – mass-spring-dashpot system – diffusion-transport cooperation – time-periodic solutions – fixed-point methods – Schauder Theorem – entropy – attractor – long time behaviour – uniqueness – logarithmic Sobolev inequality – Poincaré inequality – numerical methods for diffusions – Galerkin scheme – phase diagram

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1 Flashing ratchet – a simple model for a molecular motor

Diffusion mediated transport links together a number of seemingly unrelated phenomena such as intracellular transport in eukarya [4, 5, 31], the Janossy effect, a light actuated dye/nematic liquid crystal interaction [11, 21], and other molecular scale energy transduction processes [27]. The physical systems in which these processes take place are away from thermal equilibrium and noise plays an important role in their behavior. For that reason they are often termed *Brownian motors, molecular ratchets,* or even *Brownian ratchets* (see references in [19, 14, 30] for more details).

A common feature shared by these systems is the cooperation of two opposing tendencies: diffusion which tends to spread and dissipate density and transport which concentrates density at specific sites determined by the energy landscape. The result of this collaboration is *unidirectional transport of mass.* This is in spite of the fact that each of the component processes, diffusion and transport, is spatially unbiased. Acting separately there is no mean net transport of mass. Diffusion mediated transport is therefore a transient cooperation of two opposing phenomena. Explaining unidirectional transport in Brownian motors involves understanding of their intermediate dynamics and metastable environment.

We begin by considering the following Fokker-Planck type problem

$$\begin{array}{ll} u_t = (\sigma u_x + \psi_x u)_x, & (x,t) \in \Omega \times (0,\infty), \\ \sigma u_x + \psi_x u = 0, & (x,t) \in \partial\Omega \times (0,\infty), \\ u(x,0) = u_0(x), & x \in \Omega, \end{array} \tag{1}$$

where $\sigma > 0$, $u_0 > 0$, $\int_\Omega u_0 = 1$ and the potential $\psi = \psi(x,t)$ is a periodic function of t. For simplicity we assume that $\Omega = (0,1)$. Many of our results apply when Ω is a bounded domain in $\mathbb{R}^N$, $N \geq 1$, however the one dimensional case seems to be the most important in applications. Notice that if $u(x,0) = u_0 > 0$ then $u(x,t) > 0$ for all $t > 0$. Also if $\int_\Omega u_0 = 1$ then $\int_\Omega u(x,t)\,dx = 1$. Thus (1) in general can be thought of an evolution equation for probability density u. With an appropriate time rescaling, σ can be supposed equal to 1.

For the special case when ψ oscillates between a periodic, asymmetric k-well potential (see Figure 1) and $\psi \equiv 0$, (1) is called the *flashing ratchet.* To explain how the flashing ratchet works imagine an assembly of particles on the interval Ω with the potential ψ acting on them. During the transport phase ($T_{\rm tr}$) the potential is switched on and most of the particles "slide down" the potential wells with much smaller fraction of them "jumping", thanks to diffusion, across the energy barrier. When the potential is switched off ($T_{\rm diff}$) particles are subject only to random fluctuations resulting in Brownian motion which, on the mesoscopic level, manifests itself as diffusion. It is important to keep in mind that in the infinite limit of the "off" phase the particles would be uniformly distributed; likewise in the infinite limit of the "on" phase the particles would be distributed in equal portions among the wells of the potential (see Figure 1 where the Gibbs distribution is shown). In either case no transport of mass can be observed.

However, not immediately obvious but intuitively clear is the fact that the flashing ratchet may induce transport of particles in a specific, preferred direction and thus could serve as a "caricature" for understanding the energy transduction of a Brownian motor. Indeed, this exact description has been proposed as the mechanism for the KIF-1A family of motor proteins [23, 24].

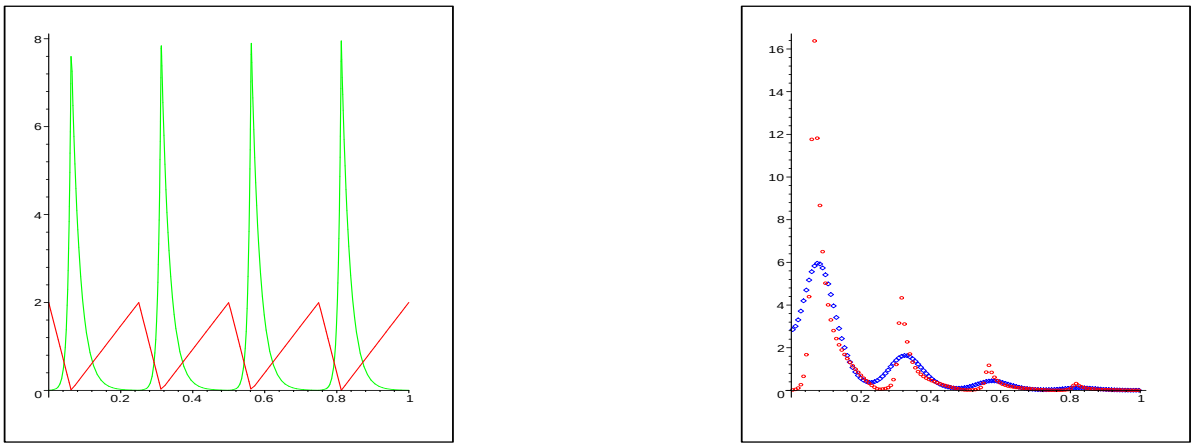

Figure 1: *A periodic asymmetric potential ψ and its Gibbs distribution (left) and the periodic state at two different instants (right).*

We should point out here that, in addition to *diffusion-transport cooperation* mentioned, one more important feature of the motion of the molecular motors is that it takes place in a viscous environment and thus it is reasonable to think of it as *overdamped motion.* In this paper we introduce the minimum energy dissipation principle by which the flashing ratchet model is derived for an assembly of particles moving in the viscous environment. This gives further validity for application of the ratchet type models in the context of intracellular dynamics. It is reinforced by the fact that more complicated models for molecular motors that also account for chemically based conformational changes [1, 18, 28, 29], can be derived using the same minimum dissipation principle [9]. The dissipation principle establishes the weak topology as the ambient space for the system.

In [19] the second and the third authors established rigorously that the unidirectional transport indeed takes place for the appropriately "tuned" two well flashing ratchet. More generally, they showed that for a range of parameters $T_{\rm tr}, T_{\rm diff}$ and σ there is a unique periodic orbit U for (1), which is asymptotically stable and thus it represents the long time behavior of the flashing ratchet. In order to describe the transfer of mass between the wells of the potential during one cycle $T = T_{\rm tr} + T_{\rm diff}$ a Markov chain was introduced. This Markov chain approximates the flashing ratchet in the sense of weak topology. In the present paper we propose yet another approximation based on the minimum energy dissipation principle. The difference between the two is that the new approximation is discrete in space and (unlike the Markov chain) continuous in time. Another objective of the present paper is to generalize those results to a wide class of potentials (for example we drop the assumptions on $T_{\rm tr}, T_{\rm diff}$) and also provide more precise information about the (exponential) rate at which the trajectories converge to U.

This paper is organized as follows: we first show that the flashing ratchet model can be derived by the mean of a minimum dissipation principle, following [9]. Our next goal is to prove the existence of periodic solutions to (1). We will also study their stability and prove an

exponential rate of convergence of the solutions of the evolution problem to the time-periodic ones. We will then give an interpretation of the flashing ratchet through a discretization scheme that sheds a new light on the dynamics of systems like (1). In this paper, we will not cover the most general situation but rather consider cases of interest for molecular motors.

2 Minimum energy dissipation principle

In this section we present the argument developed in [9] and also follow the ideas developed by Jordan, Kinderlehrer and Otto [17].

2.1 Review of the Wasserstein distance

We recall that the Wasserstein distance between two Borel probability measures μ, μ^* is defined as

$$d(\mu,\mu^*)^2 = \inf_{p\in\mathcal{P}(\mu,\mu^*)} \int_{\Omega\times\Omega} |x-\xi|^2\, p(dxd\xi), \tag{2}$$

where $\mathcal{P}(\mu,\mu^*)$ is the set of probability measures in $\Omega\times\Omega$ with marginals μ and μ^*. It induces the weak* topology on the measures.

Assume that μ, μ^* are measures with densities, respectively, f, f^*. Further suppose that there is a strictly increasing continuous mapping $\phi:\Omega\to\Omega$, $\phi(0)=0$, $\phi(1)=1$ such that

$$\int_\Omega \zeta\, f\, d\xi = \int_\Omega \zeta(\phi(x))\, f^*(x)\, dx, \qquad \text{for any } \zeta\in C^0(\Omega).$$

We say that f is the push forward of f^* and ϕ is the associated transfer function. In particular if ζ is a characteristic function of the interval $[0,x]$, then

$$\int_0^{\phi(x)} f(\xi)\, d\xi = F(\phi(x)) = \int_0^x f^*(x')\, dx' = F^*(x),$$

where F, F^* are the distribution functions of f, f^*. Thus in one dimension the unique transfer function can be determined through the formula $\phi(x)=F^{-1}(F^*(x))$. The Wasserstein distance between $f\,d\xi$ and f^*dx can be expressed in terms of ϕ by the formula

$$d(f,f^*)^2 = \int_\Omega |x-\phi(x)|^2 f^*(x)\, dx.$$

We will now present yet another formula equivalent to (2) that was derived by Benamou and Brenier [7] and involves a convex duality. Let densities $f(\xi,t)$, $0\le t\le\tau$ and $f^*(x)$ be given and let $\phi(x,t)$ be the associated transfer function, *i.e.*,

$$\int_\Omega \zeta(\xi)\, f(\xi,t)\, d\xi = \int_\Omega \zeta(\phi(x,t))\, f^*(x)\, dx, \quad \text{for any } \zeta\in C^0(\Omega), \quad 0\le t\le\tau.$$

We assume that for any t, $\phi(\cdot,t)$ is continuous and strictly increasing with respect to x. From this it follows

$$\int_0^{\phi(x,t)} f(\xi)\, d\xi = \int_0^x f^*(x')\, dx',$$

which, upon differentiating with respect to t and x yields

$$f_\xi(\phi(x,t),t)\,\frac{\partial\phi}{\partial t}\frac{\partial\phi}{\partial x}+f_t(\phi(x,t),t)\,\frac{\partial\phi}{\partial x}+f(\phi(x,t),t)\,\frac{\partial^2\phi}{\partial x\partial t}=0.$$

We implicitly define a velocity ν by

$$\nu(\phi,t)=\frac{\partial\phi}{\partial t}.$$

Using $\frac{\partial^2\phi}{\partial x\partial t}=\nu_\xi(\phi,t)\frac{\partial\phi}{\partial x}$ we find a continuity equation for $f(x,t)$:

$$f_t+(\nu f)_x=0,\qquad \text{in } \Omega\times(0,\tau).$$

The result of [7] states that given an initial density f^* and a final one f^{**},

$$d(f^{**},f^*)^2=\tau\min_\nu\int_0^\tau\int_\Omega\nu(x,t)^2f(x,t)\,dxdt,$$

where the minimum is taken over all velocities ν such that

$$\begin{array}{ll} f_t+(\nu f)_x=0, & \text{in } \Omega\times(0,\tau),\\ f(x,0)=f^*,\quad f(x,\tau)=f^{**}(x) & x\in\Omega. \end{array}\tag{3}$$

We note that there are very similar considerations in [25] and [26].

2.2 Mass-spring-dashpot system

A simple mechanical analog of a molecular motor is a mass-spring-dashpot system. We refer the reader to [16] where, based on this idea, various mechanical properties of molecular motors are discussed. In particular, it is pointed out there that in general molecular motors move in a very viscous environment and consequently damping is an important effect and kinetic energy is insignificant.

Recall that the motion of a damped spring with mass m, spring constant k and damping coefficient γ is governed by the well known ODE

$$\begin{array}{ll} m\,\xi''+\gamma\,\xi'+k\,\xi=0, & 0<t\le\tau,\\ \xi(0)=x,\quad \xi'(0)=v. & \end{array}$$

The conservation of energy (kinetic, potential and dissipated due to damping) gives the relation

$$\frac12\,m\,|\xi'(\tau)|^2+\gamma\int_0^\tau|\xi'(t)|^2\,dt+\frac{k}{2}\,|\xi(\tau)|^2=const.$$

Now consider an overdamped system $\gamma\gg mk$. Suppose that an assembly of springs is initially distributed in Ω with density $f^*(x)$. We define $\phi(x,t)=\xi(t)$. The energy dissipated in the system is then

$$\delta=\gamma\int_0^\tau\int_\Omega\phi_t(x,t)^2f^*(x)\,dxdt.$$

Let the transported density $f(\xi,t)$ be defined by

$$\int_\Omega\zeta(\xi)\,f(\xi,t)\,d\xi=\int_\Omega\zeta(\phi(x,t))\,f^*(x)\,dx,\qquad \text{for any } \zeta\in C^0(\Omega),\ 0\le t\le\tau,$$

with terminal distribution $f(x,\tau) = f^{**}$. Setting $\nu(x,t) = \phi_t(x,t)$ we see that $f(x,t)$ satisfies the continuity equation (3) and

$$\delta = \gamma \int_0^\tau \int_\Omega |\nu(x,t)|^2 f(x,t)\, dxdt \geq \gamma \min_\nu \int_0^\tau \int_\Omega |\nu(x,t)|^2 f(x,t)\, dxdt = \frac{\gamma}{\tau}\, d(f^{**}, f^*)^2.$$

2.3 Variational Principle for the Fokker-Planck equation

We introduce the free energy functional

$$F(u) = \int_\Omega (\psi\, u + \sigma\, u \log u)\, dx.$$

In [17] the following implicit scheme for solving (1) is introduced: Determine $u^{(k)}$ such that

$$\frac{1}{2} d(u^{(k-1)}, u^{(k)})^2 + \tau F(u^{(k)}) = \min_u \left[\frac{1}{2} d(u^{(k-1)}, u)^2 + \tau F(u) \right]. \tag{4}$$

Let the approximating solution $u_\tau(t)$ be defined by interpolation:

$$u_\tau(x,t) = u^{(k)}(x) \quad \text{if } t \in [k\,\tau, (k+1)\,\tau),\ x \in \Omega.$$

The main results of [17] can be summarized as follows:

(1) There exists a unique solution to the above scheme.

(2) As $\tau \to 0$, u_τ converges strongly in $L^1((0,t) \times \Omega)$ to the unique solution to (1) (see Section 5 for more details).

The preceding discussion, in which we interpreted the Wasserstein distance as the minimum of the energy dissipated in the mass-spring-dashpot system due to friction, together with (4) mean that the evolution process governed by the Fokker-Planck equation follows the path of minimum dissipation of the total energy in the weak* topology.

Observe that in the limit $\tau \to 0$, by (4) and [7], the solution $u(x,t)$ of (1) will satisfy

$$\frac{d}{dt} F(u(\cdot,t)) = -\int_\Omega |\nu(x,t)|^2\, u(x,t)\, dx$$

where $\nu(x,t)$ is the optimal velocity field. A direct computation using (1) shows that

$$\frac{d}{dt} F(u(\cdot,t)) = -\int_\Omega u\ |(\sigma \log u + \psi)_x|^2\ dx,$$

which suggests that $\nu(x,t) = -(\sigma \log u + \psi)_x$. This is actually the case, as we shall see in Section 5.1.

Given the flashing ratchet as a model for molecular motors we see that this principle as a possible general rule governing molecular scale energy transduction processes. This postulate is further suggested by the fact that more complicated (and more realistic) two state models for molecular motors can be interpreted within the same energy dissipation framework [9].

In the last section of the present paper we will consider the energy dissipation principle once again and show that it gives rise to a novel Galerkin scheme for the Fokker-Planck type problem. This scheme is not only relevant from the point of view of numerical calculations but also gives some insight into the mechanism of mass transport in the flashing ratchet.

3 Periodic state and asymptotic behaviour

We first state an existence result for periodic solutions. Henceforth, we set the diffusion constant $\sigma = 1$.

Theorem 1 *Let $\psi \in L^\infty([0,T)\times\Omega)$ be a T-periodic potential and assume that there exists a finite partition of $[0,T)$ into intervals $[T_i,T_{i+1})$, $i=0,...,n$ with $T_0=0$, $T_n=T$ such that $\psi_{[T_i,T_{i+1})}\in L^\infty([T_i,T_{i+1}),W^{1,\infty}(\Omega))$. Then there exists a unique nonnegative T-periodic solution U to (1) such that $\int_\Omega U(x,t)\,dx=1$ for any $t\in[0,T)$.*

The proof holds not only for an interval $\Omega\subset\mathbb{R}$ but also for an arbitrary bounded domain $\Omega\subset\mathbb{R}^N$ with, for instance, C^1 by parts boundary conditions (assuming of course that u satisfies the natural boundary conditions). Let

$$\sigma_q(u)=\begin{cases}\frac{u^q-1}{q-1} & \text{if } q>1,\\ u\ln u & \text{if } q=1.\end{cases}$$

Notice that σ_q is strictly convex.

We define the entropy and the entropy production respectively by

$$\Sigma_q[u|v]=\int_\Omega\left[\sigma_q\left(\frac{u}{v}\right)-\sigma_q'(1)\left(\frac{u}{v}-1\right)\right]v\,dx$$

and

$$I_q[u|v]=\int_\Omega\sigma_q''\left(\frac{u}{v}\right)\left|\nabla\left(\frac{u}{v}\right)\right|^2 v\,dx,$$

for nonnegative functions u and v.

Since (1) is linear, we have not imposed any restriction by assuming that $\int_\Omega u_0\,dx=1$. Because of the boundary conditions, it is clear that for any solution of (1), $\int_\Omega u(x,t)\,dx=1$, for any $t>0$. Also notice that $\Sigma_q[u|v]=\int_\Omega\sigma_q\left(\frac{u}{v}\right)v\,dx$ for any nonnegative functions u and v such that $\int_\Omega u\,dx=\int_\Omega v\,dx=1$. From now on, we shall assume without further notice that all functions are normalized to 1 in $L^1(\Omega)$.

In the important case when $q=1$ the expressions for Σ_1 and I_1 can be written in a more transparent form:

$$\begin{aligned}\Sigma_1[u|v] &= 2\int_\Omega\left(\frac{u}{v}\right)\ln\left(\frac{u}{v}\right)^{1/2}v\,dx,\\ I_1[u|v] &= 4\int_\Omega\left|\nabla\left(\frac{u}{v}\right)^{1/2}\right|v\,dx.\end{aligned}$$

The key here is that the relative entropy and entropy production can be expressed as functions of $w=\frac{u}{v}$ integrated with respect to $v\,dx$.

The uniqueness of the periodic orbit as well as the exponential decay of any solution to the unique periodic solution follows from the next theorem.

Theorem 2 *Let u_1,u_2 be any two solutions to (1). Under the same conditions as in Theorem 1, it holds that*

$$\Sigma_q[u_1(t)|u_2(t)]\le e^{-C_qt}\Sigma_q[u_1(0)|u_2(0)],$$

where the constant $C_q>0$ depends on q only and will be specified later.

This contraction property is true not only in the entropy sense, but also in $L^q(\Omega)$. For completeness, we reproduce here a result which is stated in the whole space case in [8]. The adaptation of the proof is left to the reader. The case $q = 1$ is the well known Csiszár-Kullback inequality (see for instance [10, 22, 2]) and the case $q = 2$ is trivial.

Proposition 3 *Assume that Ω is a bounded domain in $\mathbb{R}^d$ with C^1 boundary. Let u and v be two nonnegative functions in $L^1 \cap L^q(\Omega)$ if $q \in (1, 2]$ and in $L^1(\Omega)$ with $u \log u$ and $u \log v$ in $L^1(\Omega)$ if $q = 1$. Then the following inequality holds:*

$$\Sigma_q[u|v] \geq 2^{-2/q} q \left[\max\left(\|u\|^{2-q}_{L^q(\Omega)}, \|v\|^{2-q}_{L^q(\Omega)}\right)\right]^{-1} \|u - v\|^2_{L^q(\Omega)}.$$

Although this is quite straightforward, the asymptotic behaviour of any solution of (1) is completely described as a consequence of Theorem 1, Theorem 2 and Proposition 3.

Corollary 4 *Let $q \in [1, 2]$. Under the assumptions of Theorem 1, there exists a constant $C_{q,\psi} > 0$ such that any solution of (1) corresponding to a non trivial initial data $u_0 \in L^1 \cap L^q(0, 1)$, with $u_0 \log u_0 \in L^1(0, 1)$ if $q = 1$, converges to $\|u_0\|_{L^1} U(x, t)$, where U is the periodic solution found in Theorem 1, according to*

$$\Big\|u(x,t) - \|u_0\|_{L^1} U(x,t)\Big\|_{L^q(0,1;dx)} \leq K\, e^{-C_{q,\psi}\, t} \quad \forall\, t \geq 0$$

for some constant $K = K(\max_{t\geq 0} \|u(\cdot, t)\|_{L^q}) > 0$.

The only difficulty has to do with the constant K, which depends on $\max_{t\geq 0} \|u(\cdot, t)\|_{L^q}$ and is therefore not known in an explicit form, except in the case $q = 1$.

The existence of the unique periodic orbit (Theorem 1) and the exponential decay (Theorem 2) depend on establishing estimates of the form $\Sigma_q[u|v] \leq C I_q[u|v]$. These in turn are consequences of *convex Sobolev inequalities,* which can be explained as follows. Assume first that in the definition of σ_q we take $q = 2$. We then have

$$\Sigma_2[u|v] = \int_\Omega \left(\frac{u}{v} - 1\right)^2 v\, dx\,, \quad I_2[u|v] = 2 \int_\Omega \left|\nabla\left(\frac{u}{v}\right)\right|^2 v\, dx.$$

Thus in the case $q = 2$ one expects to have an estimate $\Sigma_2[u|v] \leq C\, I_2[u|v]$. This is actually nothing else but the *weighted Poincaré inequality.*

In the other extreme case, *i.e.* $q = 1$, we have

$$\Sigma_1[u|v] = \int_\Omega u \log\left(\frac{u}{v}\right) dx = 2 \int_\Omega \left[\left(\frac{u}{v}\right)^{1/2}\right]^2 \log\left(\frac{u}{v}\right)^{1/2} v\, dx,$$

while

$$I_1[u|v] = 4 \int_\Omega \left|\nabla\left(\frac{u}{v}\right)^{1/2}\right|^2 v\, dx.$$

The estimate $\Sigma_1[u|v] \leq C I_1[u|v]$ is known as the *logarithmic Sobolev inequality* for the measure $v\, dx$. The next Theorem shows that for the whole range of $1 \leq q \leq 2$ required estimates hold true.

Let $\mathcal{X}$ be the set of bounded nonnegative functions u in $L^1 \cap L^q(\Omega)$ (resp. in $L^1(\Omega)$ with $u \log u$ in in $L^1(\Omega)$) if $q \in (1, 2]$ (resp. if $q = 1$) such that $\int_\Omega u\, dx = 1$.

Theorem 5 *Assume that* $v \in \mathcal{X}$ *with* $0 < m := \inf_\Omega v \le v \le \sup_\Omega v =: M < \infty$. *For any* $q \in [1,2]$

$$\mathcal{I} = \frac{q}{q-1} \inf_{\substack{u \in \mathcal{X} \\ u \neq v \text{ a.e.}}} \frac{I_q[u|v]}{\Sigma_q[u|v]} \quad \text{if } q > 1 \quad \text{and} \quad \mathcal{I} = \inf_{\substack{u \in \mathcal{X} \\ u \neq v \text{ a.e.}}} \frac{I_1[u|v]}{\Sigma_1[u|v]} \quad \text{if } q = 1 \tag{5}$$

can be estimated by

$$\mathcal{I} \ge 4\,\lambda_1(\Omega)\,\frac{m}{M} \tag{6}$$

where $\lambda_1(\Omega)$ *is Poincaré's constant of* Ω *(with weight* 1*).*

In the above inequality, $\lambda_1(\Omega)$ denotes the first eigenvalue of the Laplacian with zero Neumann boundary conditions:

$$\lambda_1(\Omega) := \inf_{w \in H^1(\Omega)} \frac{\|\nabla w\|^2_{L^2(\Omega)}}{\|w - \bar{w}\|^2_{L^2(\Omega)}}$$

where $\bar{w} = \frac{1}{|\Omega|}\int_\Omega w(x)\,dx$ is the average of w.

Convex Sobolev inequalities relating I_q and Σ_q have been extensively studied by entropy-entropy production methods (see [3] and references therein) in $\Omega = \mathbb{R}^N$ (also see [13, 6]). This method also applies in a bounded domain Ω provided it is convex. Here we prove it as a direct consequence of the standard Poincaré inequality (with weight 1) using a perturbation approach inspired by the Holley-Stroock lemma (see [15, 3]).

4 Proofs

This section is devoted to the proofs of the results of Section 1. We shall first prove the existence of a periodic solution to (1) using the entropy Σ_1 (Theorem 1) by a fixed-point method. Then we prove Theorem 5 and get the exponential decay of the entropy Σ_q for any $q \in [1,2]$.

4.1 Existence of periodic solutions

In the sequel we will denote:

$$u_\psi(x,t) = \frac{e^{-\psi(x)}}{\int_\Omega e^{-\psi(y)}dy},$$

where ψ is the potential in (1).

For simplicity, we will only deal with two cases corresponding to smooth potentials or to *flashing potentials* with two time subintervals only, on which the potentials are smooth. Here *smooth* means that

$$K_\psi = \sup_{0 \le t < T} \left\| \frac{u_{\psi,t}}{u_\psi} \right\|_{L^\infty(\Omega)}$$

is bounded. Note that $K_\psi = \|\psi_t\|_{L^\infty(\Omega \times [0,T))}$. Our goal is to prove that there exists a periodic solution to (1). The generalization which gives the results of Theorem 1 is then easy and left to the reader. The uniqueness is a consequence of Theorem 2. Let

$$C_\psi = 4\lambda_1(\Omega) \inf_{0 \le t < T} e^{\mathcal{V}(\psi(\cdot,t))}$$

where $\mathcal{V}(\phi) := \max_\Omega \phi - \min_\Omega \phi$ is the total oscillation of ϕ. With the notations of Theorem 5, if $v = u_\psi$, then $e^{\mathcal{V}(\psi(\cdot,t))} = e^{\mathcal{V}(\psi(\cdot,t) - \log(\int_\Omega \psi(x,t)\,dx))} = \frac{m}{M}$.

4.1.1 Smooth potentials

Lemma 6 *Let $u \geq 0$ be a solution to (1) such that $\int_\Omega u\,dx = 1$. With the above notations, the following estimate holds:*

$$\frac{d}{dt}\Sigma_1[u|u_\psi] \leq -C_\psi\,\Sigma_1[u|u_\psi] + K_\psi. \tag{7}$$

Proof. Calculating directly we have

$$\begin{aligned}
\frac{d}{dt}\Sigma_1[u|u_\psi] &= \frac{d}{dt}\int_\Omega u \log\left(\frac{u}{u_\psi}\right) dx \\
&= \int_\Omega \left[1 + \log\left(\frac{u}{u_\psi}\right)\right] u_t\,dx - \int_\Omega \frac{u}{u_\psi}\,u_{\psi,t}\,dx \\
&= -I_1[u|u_\psi] - \int_\Omega \frac{u}{u_\psi}\,u_{\psi,t}\,dx \\
&\leq -C_\psi\,\Sigma_1[u|u_\psi] + K_\psi
\end{aligned}$$

according to (6). □

Proof of Theorem 1 (smooth potentials). We will show that the map $\mathcal{T}(u(\cdot,0)) = u(\cdot,T)$ has a fixed-point in a suitable set. This is equivalent to the existence part of our theorem. Let

$$\mathcal{Y} = \{u \in H^1(\Omega) \mid u \geq 0\,,\ \|u\|_{L^1(\Omega)} = 1\,,\ \Sigma_1[u|u_0(\cdot,0)] \leq K_\psi/C_\psi\}.$$

We observe that $\mathcal{Y}$ is a closed and convex subset of $H^1(\Omega)$. By the Schauder Fixed-Point Theorem it suffices to show that:

(a) $\mathcal{T}(\mathcal{Y}) \subset \mathcal{Y}$

(b) The mapping $\mathcal{T}$ is compact.

(b) follows by parabolic regularity. To establish (a) we apply Lemma 6. Multiplying estimate (7) by $e^{C_\psi t}$, integrating over the interval $(0,T)$ and using periodicity of u_0 we get:

$$\Sigma_1[u|u_0]_{|t=T} \leq \Sigma_1[u|u_0]_{|t=0} e^{-C_\psi T} + K_\psi(1 - e^{-C_\psi T})/C_\psi \leq K_\psi/C_\psi.$$

Thus $\mathcal{T}$ has a fixed-point in $\mathcal{Y}$. □

4.1.2 Flashing potentials

We will now assume that

$$\psi(x,t) = \begin{cases} \psi_1(t,x) & \text{if } 0 \leq t < T_1, \\ \psi_2(t,x) & \text{if } T_1 \leq t < T_1 + T_2 \equiv T, \end{cases} \tag{8}$$

and ψ is periodic with period T. A special case is the *flashing ratchet,* where ψ_1 is sawtooth-like and asymmetric in each basin (See Section 5.2 for an example) which does not depend on t and $\psi_2 \equiv 0$. We now have to modify the argument from the previous section taking into account the fact that ψ, hence u_ψ is not differentiable with respect to t. Let $u_{\psi,1} = u_{\psi_{|t\in[0,T_1)}}$ and $u_{\psi,2} = u_{\psi_{|t\in[T_1,T_2)}}$.

Using Lemma 6 we get

$$\Sigma_1[u|u_{\psi,1}]\,|_{t=T_1} \;\le\; \Sigma_1[u|u_{\psi,1}]\,|_{t=0}\; e^{-C_{\psi_1}T_1} + \frac{K_{\psi_1}(1-e^{-C_{\psi_1}T_1})}{C_{\psi_1}}, \tag{9}$$

$$\Sigma_1[u|u_{\psi,2}]\,|_{t=T} \;\le\; \Sigma_1[u|u_{\psi,2}]\,|_{t=T_1}\; e^{-C_{\psi_2}T_2} + \frac{K_{\psi_2}(1-e^{-C_{\psi_2}T_2})}{C_{\psi_2}}. \tag{10}$$

For each nonnegative function v we have

$$\Sigma_1[v|u_{\psi,i}] = \Sigma_1[v|1] - \int_\Omega u \log u_{\psi,i}\; dx,$$

hence from (9)–(10) we get

$$\Sigma_1[u|1]\,|_{t=T} \le \Sigma_1[u|1]\,|_{t=0}\; e^{-C_{\psi_1}T_1 - C_{\psi_2}T_2} + K(\psi_1,\psi_2,T_1,T_2),$$

where $K(\psi_1,\psi_2,T_1,T_2)$ is a constant depending on ψ_1, ψ_2, T_1, T_2 only. Just like in the case of smooth potentials one can now prove the existence of a periodic orbit by considering the map $\mathcal{T}$ in the set

$$\mathcal{Y}_1 = \left\{ u \in H^1(\Omega) \mid u \ge 0\,,\ \|u\|_{L^1(\Omega)} = 1\,,\ \Sigma_1[u|1] \le \frac{K(\psi_1,\psi_2,T_1,T_2)}{1-e^{-C_{\psi_1}T_1 - C_{\psi_2}T_2}} \right\}$$

This ends the proof of Theorem 1 in the case of flashing potentials corresponding to (8). □

4.2 Poincaré type inequalities

Proof of Theorem 5. Consider first the case $q \in (1,2]$. Both numerator and denominator in (5) are homogeneous of order q in u (replacing u by $\mu\, u$ for some $\mu > 0$ means that $\Sigma_q[u|v]$ and $I_q[u|v]$ are multiplied by μ^q, so it is not restrictive to further assume that $\|u\|_{L^1(\Omega)} = 1$. Let $w = (\frac{u}{v})^{q/2}$.

$$I_q[u|v] = \frac{4}{q}\int_\Omega |\nabla w|^2\; v\, dx \ge \frac{4}{q}\min_\Omega v \int_\Omega |\nabla w|^2\; dx.$$

Applying the Poincaré inequality, we get

$$\int_\Omega |\nabla w|^2\; dx \ge \lambda_1(\Omega) \int_\Omega |w-\bar w|^2\; dx$$

with $\bar w = \frac{1}{|\Omega|}\int_\Omega w(x)\, dx$. One also has

$$\int_\Omega |w-\bar w|^2\; dx \ge (\max_\Omega v)^{-1} \int_\Omega |w-\bar w|^2\; v\, dx.$$

Let $\tilde w = \int_\Omega w\ v\,dx$. Using $\int_\Omega v\,dx = 1$, we get

$$\begin{aligned}\int_\Omega |w-\bar w|^2\ v\,dx &= \int_\Omega |w-\tilde w+\tilde w-\bar w|^2\ v\,dx\\ &= \int_\Omega |w-\tilde w|^2\ v\,dx + \int_\Omega |\tilde w-\bar w|^2\ v\,dx\\ &\ge \int_\Omega |w-\tilde w|^2\ v\,dx = \int_\Omega w^2\ v\,dx - \tilde w^2\end{aligned}$$

since $\int_\Omega (w-\tilde w)\ v\,dx = 0$ and $\int_\Omega w\,\tilde w\ v\,dx = \tilde w^2 \int_\Omega v\,dx = \tilde w^2$ by definition of $\tilde w$. On the one hand,

$$\int_\Omega w^2\ v\,dx = \int_\Omega \left(\frac{u}{v}\right)^q\ v\,dx,$$

and on the other hand,

$$\tilde w = \int_\Omega w\ v\,dx = \int_\Omega u^{q/2}\ v^{1-q/2}\,dx \le \left(\int_\Omega u\ dx\right)^{q/2} \left(\int_\Omega v\ dx\right)^{1-q/2} = 1$$

by Hölder's inequality (note that $1 < q \le 2 \iff 1 \le 2/q < 2$). Thus

$$\int_\Omega |w-\bar w|^2\ v\,dx \ge \int_\Omega \left[\left(\frac{u}{v}\right)^q - 1\right]\ v\,dx = (q-1)\,\Sigma_q[u|v].$$

Collecting the above estimates, we obtain

$$I_q[u|v] = \frac{4}{q}\,\lambda_1(\Omega)\,\frac{\min_\Omega v}{\max_\Omega v}\,(q-1)\,\Sigma_q[u|v],$$

which proves Inequality (6) and gives the positivity of $\mathcal{I}$ for any $q \in (1,2]$.

If $q = 1$, as above, by homogeneity of order 1, we may replace u and v respectively by $\mu\,u$ and $\mu\,v$ for some $\mu > 0$, in order that $\int_\Omega v\,dx = 1$. Then, with $\mu = \|u\|_{L^1(\Omega)}$, $I_1[u|v] = \mu\,I_1[\mu^{-1}u|v]$ and $\Sigma_1[u|v] = \mu\,\Sigma_1[\mu^{-1}u|v] + \mu\log\mu - (\mu-1)$. Since $\mu \mapsto \mu\log\mu - (\mu-1)$ reaches its maximum on $(0,+\infty)$ for $\mu = 1$, we may again assume that $\|u\|_{L^1(\Omega)} = 1$. At least for a sufficiently smooth function u,

$$\lim_{q\to 1} I_q[u|v] = I_1[u|v] \quad\text{and}\quad \lim_{q\to 1} \frac{1}{q-1}\,\Sigma_q[u|v] = \Sigma_1[u|v],$$

which proves Inequality (6) if $q = 1$ for any u, by a density argument. □

4.3 Exponential decay of the entropy

Proof of Theorem 2. We set $v = u_1/u_2$. Calculating directly we have

$$\frac{d}{dt}\Sigma_q[u_1|u_2] = \int_\Omega \sigma_q'(v)\,u_{1,t}\ dx + \int_\Omega [\sigma_q(v) - \sigma_q'(v)v]\,u_{2,t}\ dx.$$

Using (1) and integrating by parts we get

$$\begin{aligned}\int_\Omega \sigma_q'(v)\,u_{1,t}\ dx &= -\int_\Omega \sigma_q''(v)\,(u_{1,x} + \psi_x u_1)_x\,v_x\ dx\\ &= -\int_\Omega \sigma_q''(v)\,v_x \left(\frac{u_1}{u_\psi}\right)_x u_\psi\ dx.\end{aligned}$$

A similar calculation yields

$$\int_\Omega [\sigma_q(v) - \sigma_q'(v)\, v]\, u_{2,t}\, dx = \int_\Omega \sigma_q''(v)\, v\, v_x \Big(\frac{u_2}{u_\psi}\Big)_x\, u_\psi\, dx.$$

Consequently

$$\begin{aligned}\frac{d}{dt}\Sigma_q[u_1|u_2] &= -\int_\Omega \sigma_q''(v)\, \left[v_x\Big(\frac{u_1}{u_\psi}\Big)_x - v\, v_x\Big(\frac{u_2}{u_\psi}\Big)_x\right] u_\psi\, dx\\ &= -\int_\Omega \sigma_q''(v)\, v_x^2\, u_2\, dx\\ &= -I_q[u_1|u_2].\end{aligned}$$

Using Theorem 5 we obtain the result with $C_q = (q-1)\mathcal{I}/q$ if $q \in (1,2]$ and $C_1 = \mathcal{I}$. □

5 Qualitative behaviour of the solutions: a numerical approach

5.1 A discretization of the variational principle

Motivated by the ideas in [20] Kinderlehrer and Walkington, we build a numerical scheme based on the variational principle described in Section 2. The main difficulty in implementing the scheme in dimension higher than 1 is the fact that the Wasserstein distance in dimension higher than 1 is rather difficult to approximate numerically. Recall however, in dimension 1 we have that

$$d(u,v)^2 = \int_\Omega [x - U^{-1} \circ V(x)]^2\, v(x)\, dx,$$

where U, V are the distribution functions of u, v respectively:

$$U(x) = \int_{\inf\Omega}^x u(s)\, ds\ , \quad V(x) = \int_{\inf\Omega}^x v(s)\, ds.$$

Based on this formula the implementation of the numerical scheme is rather easy.

In [20] two such implementations are suggested: one is a relaxation scheme for direct minimization and the other is a projected gradient method. Here we suggest yet another algorithm which is in fact a Galerkin scheme.

First we consider perturbations $u^\epsilon = u + \epsilon\,\xi$ where $\int_\Omega \xi = 0$. We shall also denote by $\Xi(x) = \int_{\inf\Omega}^x \xi(s)\, ds$ the antiderivative of ξ. We let $U^\epsilon = U + \epsilon\,\Xi$ be the distribution function of u^ϵ and $\varphi^\epsilon = (U^\epsilon)^{-1} \circ V$ be the transference plan between u^ϵ and v. Differentiating the relation

$$(U + \epsilon\,\Xi) \circ \varphi^\epsilon = v$$

with respect to ϵ, it is then easy to compute

$$\frac{d\varphi^\epsilon}{d\epsilon}\,|_{\epsilon=0} = -\frac{\Xi(\varphi^0)}{u(\varphi^0)}.$$

It then follows

$$\begin{aligned}\frac{1}{2}\frac{d}{d\epsilon}d(u^\epsilon,v)^2{}_{|\epsilon=0} &= \int_\Omega (x-\varphi^0)\,v\,\frac{\Xi(\varphi^0)}{u(\varphi^0)}\,dx\\ &= \int_\Omega [(\varphi^0)^{-1}-x]\,\Xi\,dx.\end{aligned}$$

We can further calculate

$$\frac{d}{d\epsilon}F(u^\epsilon)\,|_{\epsilon=0} = \int_\Omega (\log u+\psi)\,\xi\,dx$$

It follows that if for a given v, u is a minimizer of (4), then

$$\int_\Omega [(\varphi^0)^{-1}-x]\,\Xi\,dx + \tau\int_\Omega (\log u+\psi)\,\xi\,dx = 0,\quad \forall\,\Xi \quad \text{such that } \Xi'=\xi. \tag{11}$$

Notice that at this point Ξ can simply be a Lipshitz function.

We can think of u and v as density functions arising in an implicit time discretization given by the variational principle. Our goal is to recover now an "ODE" that the variational principle is a discretization of. We denote $V(x)=U^{(k-1)}$, $U=U^{(k)}$, where k represents time steps. Formally, we can write, with some first order error term W_k,

$$U^{(k)} = U^{(k-1)} + \tau W^{(k)} + o(\tau).$$

It is convenient to think of W_k as a function of $U^{(k-1)}$. The transference plan between $u^{(k-1)}$ and $u^{(k)}$, $\phi^{(k)}(x,\tau)$ satisfies

$$\frac{d}{d\tau}\left[\phi^{(k)}\right]^{-1}(\cdot,\tau)_{|\tau=0} = -\frac{W^{(k)}}{u^{(k)}}.$$

We recognize this last term as a time discretization of $\frac{U_t}{u}$. This leads to the following continuous version of (11):

$$\int_\Omega \frac{U_t}{u}\,\Xi\,dx + \int_\Omega (\log u+\psi)\,\xi\,dx = 0,\quad \forall\,\Xi \quad \text{such that } \Xi'=\xi \tag{12}$$

As noted in Section 2.3, manipulating this expression, we recover that $\nu(x,t) = -(\log u+\psi)_x$. Observe that this is also a weak form of (1) obtained in the following manner: we write (1) as

$$u_t = [u(\log u+\psi)_x]_x,$$

which upon integration becomes

$$U_t = u(\log u+\psi)_x.$$

Dividing now by u, multiplying by a test function Ξ and integrating by parts one gets (12). Clearly (12) can be derived directly from the equation (1) and this calculation remains valid whether ψ depends on t or not. Thus the weak form of (12) can be used to analyze (1). Actually, more general problems yield to the same trick, which we do not explore here. Here we chose to start from the energy considerations believing that this approach gives somehow "correct" a form of the discrete problem described in the next section. We should point out here some analogy between our approach and the one in [12].

5.2 Results of numerical simulations

Here we take $\Omega = (0,1)$. In order to discretize (12) we assume that u is approximated by a piecewise constant function with jumps at $x_j = \frac{j-1}{N}$, $j = 1, \dots, N+1$. Accordingly we set

$$u(x) = u_j \ , \quad x \in [x_j, x_{j+1}) \ , \quad j = 1, \dots, N.$$

We define test functions Ξ_j by

$$\Xi_j(x) = \begin{cases} (x - x_j) & \text{if } x \in (x_j, x_{j+1}], \\ (x_{j+2} - x) & \text{if } x \in (x_{j+1}, x_{j+2}], \\ 0 & \text{otherwise.} \end{cases}$$

We will also denote $\xi_j = \Xi_j'$. We have

$$\begin{aligned} \int_\Omega \frac{U_t}{u}\,\Xi_j\,dx &= \frac{1}{u_j}\int_{x_j}^{x_{j+1}} U_t(x - x_j)\,dx + \frac{1}{u_{j+1}}\int_{x_{j+1}}^{x_{j+2}} U_t(x_{j+2} - x)\,dx \\ &= \frac{1}{2N^2 u_j} U_t(x_{j+1}) - \frac{1}{2u_j}\int_{x_j}^{x_{j+1}} u_t (x - x_j)^2\,dx \\ &\quad + \frac{1}{2N^2 u_{j+1}} U_t(x_{j+1}) - \frac{1}{2u_{j+1}}\int_{x_{j+1}}^{x_{j+2}} u_t (x_{j+2} - x)^2\,dx \\ &= \frac{1}{2N^2} U_t(x_{j+1})\left(\frac{1}{u_j} + \frac{1}{u_{j+1}}\right) - \frac{u_{j,t}}{6N^3 u_j} + \frac{u_{j+1,t}}{6N^3 u_{j+1}}. \end{aligned}$$

Using $u_j = N[U(x_{j+1}) - U(x_j)]$ with a similar formula for u_{j+1} we get

$$\int_\Omega \frac{U_t}{u}\,\Xi_j\,dx = \frac{1}{6N^2}\left[\frac{U_t(x_j)}{u_j} + 2U_t(x_{j+1})\left(\frac{1}{u_j} + \frac{1}{u_{j+1}}\right) + \frac{U_t(x_{j+2})}{u_{j+1}}\right].$$

Straightforward calculations then lead to

$$\begin{aligned} &u_{j+1}U_t(x_j) + 2\,(u_j + u_{j+1})U_t(x_{j+1}) + u_j U_t(x_{j+2}) \\ &\qquad = 6\,N u_j u_{j+1}\left[\log\left(\frac{u_{j+1}}{u_j}\right) + (\psi_{j+1} - \psi_j)\right] \end{aligned} \tag{13}$$

Analyzing just (13) gives some insight as to the mechanism of transport in the *flashing ratchet.* To illustrate this point we consider the flashing ratchet for a 2-well potential with asymmetric wells located at 1/8 and 5/8 and in the case of a pure diffusion. To be precise, the potential is defined with the notations of Section 4.1.2 by $\psi_1(x) = 1 - 8x$ on $(0, 1/8)$, $\psi_1(x) = 8(x - 1/8)/3$ on $(1/8, 1/2)$, $\psi_1(x) = \psi_1(x - 1/2)$ on $(1/2, 1)$ and $\psi_2 \equiv 0$.

We first use a very crude spatial discretization, *i.e.*, $N = 4$. In this case we are dealing with a system of 3 equations (observe that $U(1) = \frac{1}{N}\sum_j u_j = 1$). Taking $N = 4$ is enough to capture the asymmetry of the potential although of course the results of the simulation are very inaccurate as approximation of the PDE. Nevertheless its qualitative behavior reflects the general mechanism of the flashing ratchet. Figure 2 presents results of the numerical simulations.

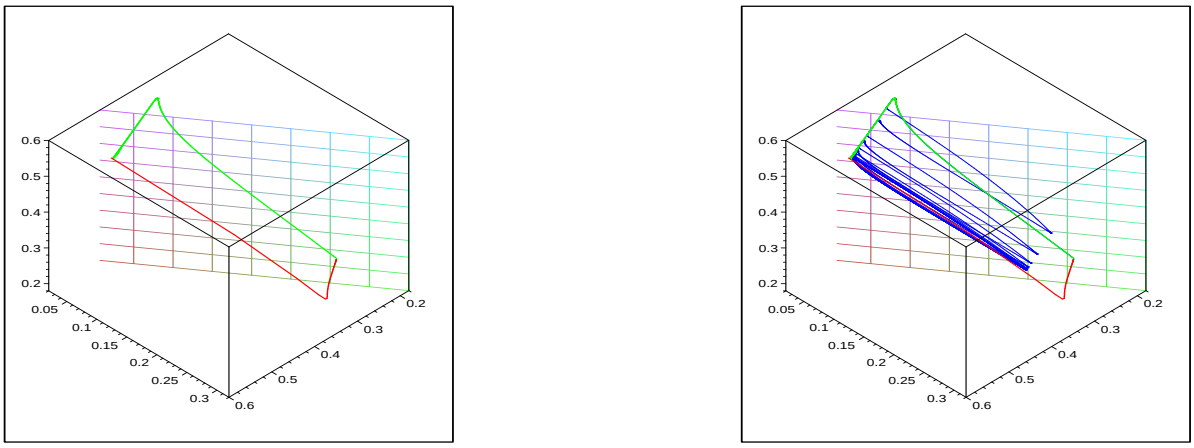

Figure 2: *Qualitative behavior of the flashing ratchet for $N = 4$. Orbits γ^+ and γ^- corresponding to pure diffusion and transport respectively (relaxation to the Gibbs state) are shown on the left. The trajectory $(u_i)_{i=1,2,3}$ is represented on the right.*

We notice that the plane Π represents the set for which the mass is equally distributed between the wells, $U(1/2) = \frac{1}{4}(u_1 + u_2) = 1/2$. Two trajectories play an important role for understanding the dynamics of (13). First is the trajectory that starts at $u_j = 1/4$, $j = 1, \dots, 3$, the stationary state of the diffusion equation. Under the Fokker-Planck flow, *i.e.*, $\psi_j \neq 0$, $j = 1, \dots, 4$ we obtain an orbit that converges asymptotically to the Gibbs distribution. Notice that during this process we have $U(1/2, t) < 1/2$, $t > 0$. We denote that orbit by γ^-.

The second trajectory lies in front of the plane $U(1/2) = 1/2$ and represents the relaxation of the Gibbs distribution by the diffusion process. Here we have $U(1/2, t) > 1/2$, $t > 0$ and this orbit is denoted by γ^+.We further notice that at first γ^+ pulls away from $U(1/2) = 1/2$ and then later turns back to follow the stable manifold of the uniform distribution. As we see on the picture on the right a typical trajectory γ oscillates near the loop formed by γ^+ and γ^-. At each cycle γ is pulled towards the set $U(1/2) > 1/2$, thanks to γ^+, and consequently more mass is accumulated. Observe that in this case most of the time the periodic orbit remains on the 'good' side of the plane Π.

Next we simulated a problem with a periodic potential with period 1/4 and 4 asymmetric wells, first one at 1/16. We took $N = 128$ and we introduced a diffusion coefficient $\sigma = 1/128$. The potential was oscillating with 4 cycles per unit time. In figure 3 we graph $U(1/2, t))$. Notice that after just few cycles $U(1/2, t) > 1/2$ throughout the whole cycle. After sufficiently long time we have $U(1/2, t) > 0.9$, which means that in the periodic state 90% of mass is concentrated in the left of the interval. One notices the loss of mass during the potential-on phase and gain during the diffusion phase. This is in the agreement with the qualitative picture we have outlined above.

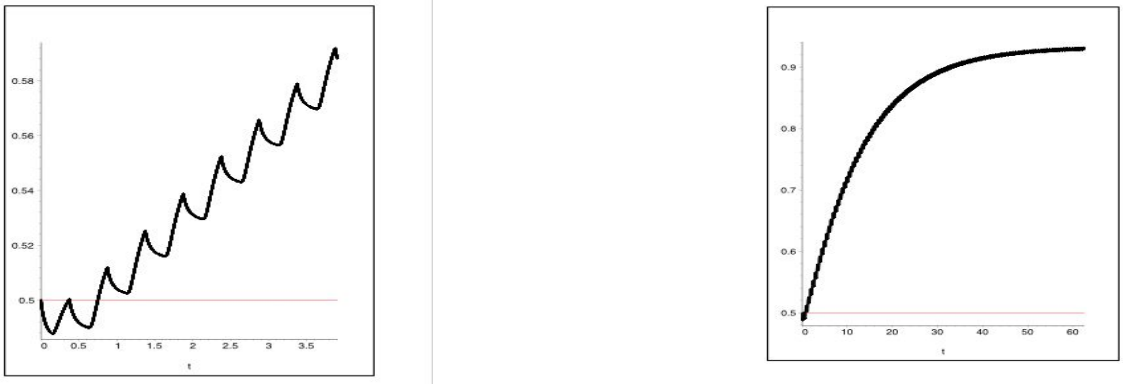

Figure 3: *Flux at 1/2 as a function of time ($N = 128$).*

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