

Remarks about the Flashing Ratchet

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Abstract

The flashing ratchet is the simplest example of diffusion mediated transport as well as the suggested mechanism for a class of protein motors. Here we briefly explain these concepts and give an entropy based argument for existence and uniqueness of a model problem. We also examine the features of the system that lead to transport.

1 Introduction

Diffusion mediated transport is involved in many mechanisms at molecular level. These include some liquid crystal and lipid bilayer systems, and, especially, the motor proteins responsible for eukaryotic cellular traffic. All of these systems are extremely complex and involve subtle interactions on various scales. In devices based on shape memory or magnetostriction, energy transduction is very close to equilibrium in order to minimize the energy budget – TV remotes are good examples. The chemical/mechanical transduction in motor proteins is, by contrast, quite distant from equilibrium. These systems function in a dynamically metastable range.

The *flashing ratchet* is, perhaps, the simplest and most transparent example of this phenomenon. It consists of apparently competing processes: a transport, which attracts mass to

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specific sites, and a diffusion, which spreads mass, in alternation. To give a simple and generalized formulation of this model, consider the following variation of the Fokker-Planck Equation:

$$\begin{cases} \rho_t = (\sigma \rho_x + \psi_x \rho)_x, & (x, t) \in \Omega \times (0, \infty), \\ \sigma \rho_x + \psi_x \rho = 0, & (x, t) \in \partial\Omega \times (0, \infty), \end{cases} \quad (1)$$

with initial data

$$\rho(x, 0) = \rho_0(x), \quad x \in \Omega,$$

where ρ_0 is nonnegative and normalized: $\int_{\Omega} \rho_0 dx = 1$. Here the diffusion coefficient σ is a positive number, the potential $\psi = \psi(x, t)$ is a periodic function of t and $\Omega = (0, 1)$. Notice that if $\rho(x, 0) = \rho_0 > 0$ then $\rho(x, t) > 0$ for all $t > 0$, and that $\int_{\Omega} \rho_0 dx = 1$ implies that $\int_{\Omega} \rho(x, t) dx = 1$. Thus (1) in general can be thought of an evolution equation for a probability density ρ .

The simplest example is given by

$$\psi(x, t) = \begin{cases} \psi(x) & \text{if } 0 \leq t \leq T_{\text{tr}}, \\ 0 & \text{if } T_{\text{tr}} \leq t \leq T_{\text{diff}} + T_{\text{tr}} = T, \end{cases} \quad (2)$$

which constitutes flashing between a diffusion with drift $\psi'(x)$ and a pure diffusion. We will refer to the time intervals $(kT, kT + T_{\text{tr}})$, $k \in \mathbb{N}$ as the *transport phase*: if σ is small, the dynamics is dominated by the drift force, and to the time intervals $(kT + T_{\text{tr}}, (k+1)T)$, $k \in \mathbb{N}$ as the *diffusion phase*. Of course, there is no stationary state for this type of equation, but there is a periodic state. The problem is interesting because the periodic state is not simply some convex combination of Gibbs states, but represents a redistribution of the mass to one side of the interval Ω , that is usually called *mass transport* (be aware that this notion has nothing to do with Monge-Kantorovich mass transport). Here our attention will focus on the existence, uniqueness, and stability of the periodic solution by employing *entropy methods*. We also discuss the approximation of the periodic state in terms of a (discrete) Markov Chain using *Monge-Kantorovich mass transport* ideas.

2 Existence and stability

We outline a simple existence and stability result. Uniqueness is a consequence of the stability. Let us assume that

$$\psi \text{ bounded and periodic of period } T \text{ in } \Omega \text{ and } \psi \in C^1(\Omega \times [0, T]).$$

Then there is a unique nonnegative T -periodic probability density $\rho = \rho^\sharp$ which solves (1).

The proof is an exercise in the use of the Schauder Fixed Point Theorem employing the free energy, a convex functional, to define the convex stable set. Let

$$E(\rho) := \int_{\Omega} \rho \log \left(\frac{\rho}{\rho_{\psi}} \right) dx \quad \text{where} \quad \rho_{\psi}(x, t) := \frac{e^{-\psi(x, t)/\sigma}}{\int_{\Omega} e^{-\psi(\xi, t)/\sigma} d\xi},$$

$$\text{for any } \rho \in H^1(\Omega), \quad \rho \geq 0, \quad \int_{\Omega} \rho dx = 1.$$

Assume that $\rho(x, t)$ is a solution of the Fokker-Planck Equation (1). Then

$$\frac{d}{dt} E(\rho(\cdot, t)) = -\sigma \int_{\Omega} \rho \left| \frac{\partial}{\partial x} \log \left(\frac{\rho}{\rho_{\psi}} \right) \right|^2 dx - \int_{\Omega} \frac{\partial \psi}{\partial t} \rho dx.$$

According to the Log-Sobolev Inequality, for a constant C_{ψ} which depends on ψ and σ ,

$$\int_{\Omega} \rho \log \left(\frac{\rho}{\rho_{\psi}} \right) dx \leq C_{\psi}^{-1} \int_{\Omega} \rho \left| \frac{\partial}{\partial x} \log \left(\frac{\rho}{\rho_{\psi}} \right) \right|^2 dx.$$

Hence, since ψ_t is bounded and ρ is a probability density for each t ,

$$\frac{d}{dt}E(\rho) \leq -\sigma C_\psi E(\rho) + K_\psi$$

and

$$E(\rho)|_{t=T} \leq E(\rho)|_{t=0} e^{-\sigma C_\psi T} + K_\psi (1 - e^{-\sigma C_\psi T}).$$

This means that the mapping

$$\begin{aligned} T : H^1(\Omega) &\rightarrow H^1(\Omega) \\ T(\rho_0)(x) &= \rho(x, T) \end{aligned}$$

where $\rho(x, t)$ is the solution of (1) with initial value ρ_0 maps the set

$$K = \left\{ \rho \in H^1(\Omega) : E(\rho) \leq \frac{K_\psi}{C_\psi} \right\} \cap \left\{ \text{probability densities} \right\}$$

into itself. The mapping T is compact by standard H^1 regularity theory for parabolic equations. Hence we obtain a fixed point ρ^\sharp of T , which is a periodic solution of (1).

We now address the stability and uniqueness of the periodic solution. We establish a decay rate for the relative entropy of two solutions of the Fokker-Planck Equation. The familiar Csiszár-Kullback Inequality or the less familiar Talagrand Inequality may then be applied. For the moment, let ρ_1 and ρ_2 be two solutions of (1). Their relative entropy at time t is

$$E(t) = E(\rho_1|\rho_2) = \int_\Omega \rho_1 \log \left(\frac{\rho_1}{\rho_2} \right) dx = \int_\Omega f \log f \rho_2 dx, \quad f = \frac{\rho_1}{\rho_2}.$$

Now compute

$$\begin{aligned} \frac{d}{dt}E(t) &= \frac{d}{dt} \int_\Omega f \log f \rho_2 dx \\ &= \int_\Omega \left\{ (\log f + 1) \left(\frac{\partial \rho_1}{\partial t} - \frac{\rho_1}{\rho_2} \frac{\partial \rho_2}{\partial t} \right) + f \log f \frac{\partial \rho_2}{\partial t} \right\} dx \\ &= \int_\Omega \log f \frac{\partial \rho_1}{\partial t} dx - \int_\Omega f \frac{\partial \rho_2}{\partial t} dx. \end{aligned}$$

Using (1) for ρ_1 and ρ_2 , we have that

$$\int_\Omega \log f \frac{\partial \rho_1}{\partial t} dx = \int_\Omega \log f \frac{\partial}{\partial x} \left(\sigma \frac{\partial \rho_1}{\partial x} + \psi_x \rho_1 \right) dx = -\sigma \int_\Omega \frac{f_x}{f} \left(\frac{\rho_1}{\rho_\psi} \right)_x \rho_\psi dx$$

and

$$-\int_\Omega f \frac{\partial \rho_2}{\partial t} dx = -\int_\Omega f \frac{\partial}{\partial x} \left(\sigma \frac{\partial \rho_2}{\partial x} + \psi_x \rho_2 \right) dx = \sigma \int_\Omega f_x \left(\frac{\rho_2}{\rho_\psi} \right)_x \rho_\psi dx.$$

Combining these identities and using $\frac{\rho_1}{\rho_\psi} = f \frac{\rho_2}{\rho_\psi}$ gives that

$$\frac{d}{dt}E(t) = -\sigma \int_\Omega \frac{f_x^2}{f} \rho_2 dx = -\sigma \int_\Omega \left| \frac{\partial}{\partial x} \log \left(\frac{\rho_1}{\rho_2} \right) \right|^2 \rho_1 dx.$$

Now again from the Log-Sobolev Inequality, if there exists an $\varepsilon > 0$ such that

$$\varepsilon \leq \rho_2 \leq \varepsilon^{-1} \quad \forall (t, x) \in \mathbb{R}^+ \times \Omega, \quad (3)$$

and if $\int_\Omega \rho_1 dx = \int_\Omega \rho_2 dx$, then

$$\int_\Omega \rho_1 \log \left(\frac{\rho_1}{\rho_2} \right) dx \leq C^{-1} \int_\Omega \left| \frac{\partial}{\partial x} \log \left(\frac{\rho_1}{\rho_2} \right) \right|^2 \rho_1 dx$$

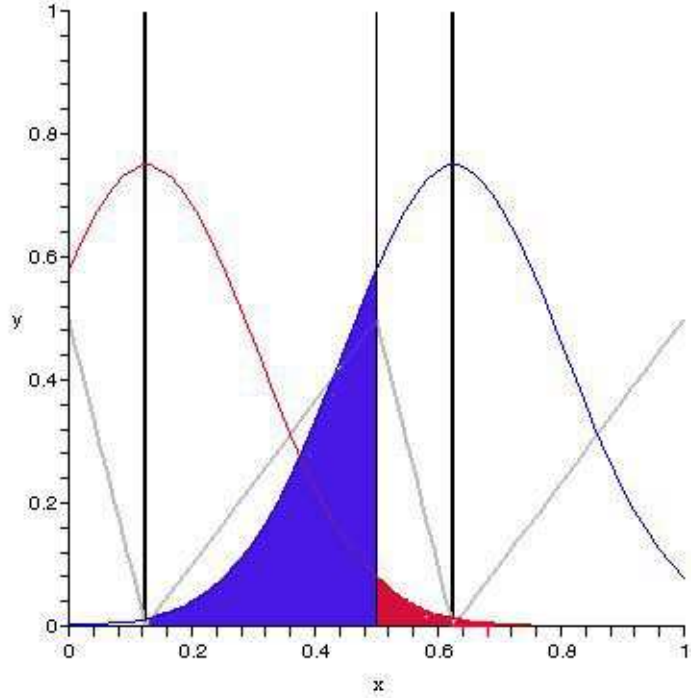


Figure 1: Two unit Dirac masses located in well basins at $x = 1/8$ and $x = 5/8$ diffuse. At the end of the diffusion period, more mass has moved to the left well from the right well than vice versa. In the ensuing transport step, more mass is collected to the well at $x = 1/8$ than to $x = 5/8$.

where C depends on ρ_2 . This can be proved by the entropy-entropy production method and a perturbation lemma (see for instance [2]). Hence,

$$E(t) \leq E(0) e^{-\sigma C t/2}, \quad t > 0.$$

At this point it is convenient to let $\rho_2 = \rho^\sharp$, the periodic solution just found. Then (3) holds and

$$\int_{\Omega} |\rho_1 - \rho^\sharp| dx \leq \text{Const.} e^{-\sigma C t/2} \quad \text{and} \quad d(\rho_1, \rho^\sharp) \leq \text{Const.} e^{-\sigma C t/2}$$

by Csiszár-Kullback and Talagrand inequalities respectively, where $d(\cdot, \cdot)$ is the Wasserstein distance. This shows both the stability and the uniqueness of the periodic solution.

As mentioned before, the extension to piecewise smooth in time potentials $\psi(x, t)$ like (2) is achieved by concatenating the estimates, e.g., by first solving a Fokker-Planck Equation and then a diffusion equation. This again proves the existence of a T -periodic solution ρ^\sharp . The contraction property and the rates of convergence measured in relative entropy are obtained exactly in the same way as before.

3 The mechanism of transport

The basic mechanism of transport may be explained with a simple picture. For this, consider (2) where $\psi(x)$ is periodic in x of period $1/N$ and between maxima has an asymmetrically located

(and unique) minimum. For example, in Figure 1, two Dirac masses located in well basins asymmetric in their period intervals diffuse for a time T_{diff} . Owing to the asymmetry alone, more mass moves to the left than to the right. In the ensuing transport step, more mass is collected in the left well than in the right one. When iterated, significant transport can result. This is misleading, however. It is important to know what to do with the mass when it arrives in the left-most well. In other words, boundary conditions are also extremely important. Periodic boundary conditions, for example, do not lead to an accumulation of mass in the most-left well – the so-called mass transport – in the flashing ratchet model. Our analysis of this Brownian motor renders the figure with boundary conditions rigorous by approximating the periodic solution ρ^\sharp with a Markov chain defined on convex combinations of Dirac masses.

Suppose that, as a typical situation, ψ has maxima at $x_0 := 0, x_1 := 1/N, \dots, x_i := i/N, \dots, x_N := 1$ and minima at a_1, \dots, a_N with $x_{i-1} < a_i < x_i$. For a solution ρ of (1), set $I_i := [x_{i-1}, x_i]$, $i = 1, \dots, N$ and define

$$\mu^* := \sum_{i=1}^N \mu_i^* \delta_{a_i} \quad \text{where } \mu_i^* = \int_{I_i} \rho(x, t) dx, \quad 0 \leq t \leq T.$$

In a moment, ρ will be the periodic solution ρ^\sharp , but for the present, if

$$\rho(x, t) \approx \mu^*$$

then

$$\rho(x, t + T) \approx \sum_{i=1}^N \mu_i^* g_\sigma(x, T, a_i) dx$$

where $g_\sigma(x, t, a)$ is Green's Function for the Neumann Problem with singularity at $x = a$ and diffusion coefficient σ . After an evolution over one time period T , we rewrite this as

$$\rho(x, t + T) \approx \mu =: \mu^* P, \quad P = (P_{ij}), \quad P_{ij} = \int_{I_j} g_\sigma(x, T, a_i) dx.$$

P is an ergodic probability matrix. Now choose $\rho = \rho^\sharp$, the periodic solution and replace the $*$ by \sharp above. Then

$$\rho^\sharp(x, 0) \approx \mu^\sharp \quad \text{and} \quad \rho^\sharp(x, T) \approx \mu^\sharp P. \quad (4)$$

Since ρ^\sharp is T -periodic, $\rho^\sharp(x, 0) = \rho^\sharp(x, T)$ implies that

$$\mu^\sharp \approx \mu^\sharp P. \quad (5)$$

The only way these iterates of a Markov chain can be close to ρ^\sharp corresponds to the case where μ^\sharp , and hence ρ^\sharp , is close to the unique stationary vector μ^∞ of P . Our strategy is to show that μ^∞ has most of its mass on one side of Ω . In summary, we find a Markov chain determined by the diffusion and the asymmetry in the system which we may attempt to exploit to characterize its transport properties. For that purpose, we will assume that the 'ratchet' parameters are appropriately tuned. We also require separate estimates for the transport and the diffusion phases. The precise distance between μ and ρ will be in weak topology, namely, expressed by the Wasserstein metric d .

First consider the transport phase. The Wasserstein distance between $\rho(x, t)$ and μ^* is nearly

$$d(\rho, \mu^*)^2 = \sum_{j=1}^N \int_{I_j} (x - a_j)^2 \rho(x, t) dx. \quad (6)$$

To determine the rate of decay of (6), differentiate with respect to t and use Equation (1). Typically this provides an exponential rate of decay by a Gronwall lemma. The estimate we obtain is

$$d\left(\rho^\sharp(\cdot, T_{\text{tr}}), \mu^\sharp\right) \leq K_0 \omega,$$

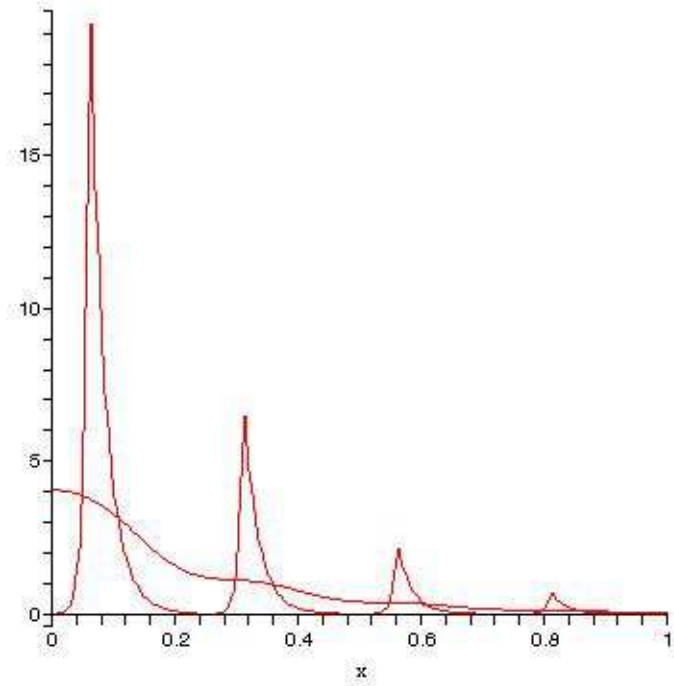


Figure 2: Snapshots of the periodic solution for a potential ψ of period $1/4$ on Ω at the end of the transport phase, upper curve, and at the end of the diffusion phase, lower curve.

where ω depends on T_{tr} , T_{diff} and σ : an explicit bound

$$\omega \leq \frac{\log T_{\text{tr}}}{T_{\text{tr}}} + \min(\sqrt{\sigma} e^{\lambda T_{\text{tr}}}, 1)$$

can be found whenever $T_{\text{tr}} \geq T_{\text{tr}}^*$, $T_{\text{diff}} \geq T_{\text{diff}}^*$, $2\pi^2\sigma T_{\text{diff}} - \lambda T_{\text{tr}} > \log 2$. Here T_{tr}^* , T_{diff}^* , K_0 and λ are all constants that depend only on the potential ψ and its derivatives. The $\log T_{\text{tr}}/T_{\text{tr}}$ term owes to the nonconvexity of the potential ψ . The second term $\min(\sqrt{\sigma} e^{\lambda T_{\text{tr}}}, 1)$ accounts for diffusion across the maxima of ψ , which is small when λT_{tr} is less than $-\log \sigma$.

During the diffusion phase, we wish to compare the two distributions $\rho(x, t)$ and $w(x, t)$, the solution of

$$\begin{aligned} w_t &= \sigma w_{xx} && \text{in } \Omega, && T_{\text{tr}} < t < T_{\text{diff}}, \\ w_x &= 0 && \text{on } \partial\Omega, && T_{\text{tr}} < t < T_{\text{diff}}, \\ w|_{t=T_{\text{tr}}} &= \sum_{i=1}^N \mu_j^\# \delta_{a_i} \end{aligned}$$

which may be accomplished in several ways. For instance, we may simply use the entropy estimate we have already proved in the previous section. This requires an estimate on $w(x, T_{\text{tr}} + \delta)$ for a small δ in order to assess $E(0)$. There are some additional details to check, but in the end, we obtain a rigorous version of (4) and (5).

Finally, we address the analysis of transport as exhibited in the Markov chain P . How do we know that the stationary vector μ^∞ of P has most of its mass in the left half of Ω when the well basins a_i are in the left halves of their intervals I_i ? Simulations show that this is clearly the case, cf. Figure 3 and even numerical calculation of μ^∞ are emphatic on this point. For the

two-well case, i.e., $N = 2$, we can verify this. In general, the slow decay of the Green's function at infinity makes estimates very difficult.

References

- [1] A. ADJARI AND J. PROST, *Mouvement induit par un potentiel périodique de basse symétrie: dielectrophorese pulse*, C. R. Acad. Sci. Paris t. **315**, Série II (1992), 1653.
- [2] A. ARNOLD, P. MARKOWICH, G. TOSCANI AND A. UNTERREITER, *On logarithmic Sobolev inequalities and the rate of convergence to equilibrium for Fokker-Planck type equations*, Comm. P.D.E. **26** no. 1-2 (2001), 43–100.
- [3] R.D. ASTUMIAN AND M. BIER, *Fluctuation driven ratchets: molecular motors*, Phys. Re. Lett. **72** (1994), 1766.
- [4] R.D. ASTUMIAN, *Thermodynamics and kinetics of a Brownian motor*, Science **276** (1997), 917–922.
- [5] W. BECKNER, *A generalized Poincaré inequality for Gaussian measures*, Proc. Amer. Math. Soc. **105** no. 2 (1989), 397–400.
- [6] J.-D. BENAMOU AND Y. BRENIER, *A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem*, Numer. Math. **84** (2000), 375–393.
- [7] M.J. CÁCERES, J.A. CARRILLO AND J. DOLBEAULT, *Nonlinear Stability in $L^p(R^d)$ for Solutions of the Vlasov-Poisson system for charged particles*, SIAM J. Math. Anal. **34** no. 2 (2002), 478–494.
- [8] M. CHIPOT, D. KINDERLEHRER AND M. KOWALCZYK, *A variational principle for molecular motors*, Meccanica, **38** (2003), 505–518
- [9] W. E AND P. PALFFY-MUHORAY, *Orientalional ratchets and angular momentum balance in the Janossy effect*, Mol. Cryst. Liq. Cryst. **320** (1998), 193–206.
- [10] T.C. ELSTON AND C.R. DOERING, *Numerical and analytical studies of nonequilibrium fluctuation-induced transport process*, Jour. Stat. Physisc **83** nos. 3/4 (1996), 359–383.
- [11] D. HEATH, D. KINDERLEHRER AND M. KOWALCZYK, *Discrete and continuous ratchets: from coin toss to molecular motor*, Discrete and continuous dynamical systems Ser. B **2** no. 2 (2002), 153–167.
- [12] R. HOLLEY, D. STROOCK, *Logarithmic Sobolev inequalities and stochastic Ising models*, J. Stat. Phys. **46** nos. 5/6 (1987), 1159–1194.
- [13] J. HOWARD, *Mechanics of Motor Proteins and the Cytoskeleton*, Sinauer Associates, Inc., 2001.
- [14] R. JORDAN, D. KINDERLEHRER AND F. OTTO, *The variational formulation of the Fokker-Planck equation*, SIAM J. Math. Anal. Vol. **29** no. 1 (1998), 1–17.
- [15] F. JÜLICHER AND J. PROST, *Cooperative molecular motors*, Phys. Rev. Lett. **75** (1995), 2618.
- [16] D. KINDERLEHRER AND M. KOWALCZYK, *Diffusion-mediated transport and the flashing ratchet*, Arch. Rat. Mech. Anal. **161** (2002), 149–179.
- [17] D. KINDERLEHRER AND N. WALKINGTON, *Approximation of parabolic equations based upon Wasserstein's variational principle*, Math. Model. Numer. Anal. (M2AN) **33** no. 4 (1999), 837–852.
- [18] T. KOSA, W. E AND P. PALFFY-MUHORAY, *Brownian motors in the photoalignment of liquid crystals*, Int. J. Eng. Science **38** (2000), 1077–1084.
- [19] Y. OKADA AND N. HIROKAWA, *A processive single-headed motor: kinesin superfamily protein KIF1A*, Science Vol. **283**, 19 February 1999.

- [20] Y. OKADA AND N. HIROKAWA, *Mechanism of the single headed processivity: diffusional anchoring between the K-loop of kinesin and the C terminus of tubulin*, Proc. Nat. Acad. Sciences **7** no. 2 (2000), 640–645.
- [21] OTTO, F., *Dynamics of labyrinthine pattern formation: a mean field theory*, Arch. Rat. Mech. Anal. **141** (1998), 63-103
- [22] OTTO, F., *The geometry of dissipative evolution equations: the porous medium equation*, Comm. PDE **26** (2001), 101-174
- [23] OTTO, F. AND C. VILLANI *Generalization of an inequality by Talagrand and links with the logarithmic Sobolev Inequality*, J. Funct. Anal. **173**, (2000), 361–400
- [24] A. VAN OUDENAARDEN AND S. BOXER, *Brownian ratchets: molecular separation in lipid bilayers supported on patterned arrays*, Science **285** (1999), 1046–1048.
- [25] A. PARMEGGIANI, F. JÜLICHER, A. ADJARI AND J. PROST, *Energy transduction of isothermal ratchets: generic aspects and specific examples close and far from equilibrium*, Phys. Rev. E, **60** no. 2 (1999), 2127–2140.
- [26] C.S. PESKIN, G.B. ERMENTROUT AND G.F. OSTER, *The correlation ratchet: a novel mechanism for generating directed motion by ATP hydrolysis*, in Cell Mechanics and Cellular Engineering (V.C Mow et.al eds.), Springer, New York, 1995.
- [27] P. REIMANN, *Brownian motors: noisy transport far from equilibrium*, Phys. Rep. **361** nos. 2–4 (2002), 57–265.
- [28] R.D. VALE AND R.A. MILLIGAN, *The way things move: looking under the hood of motor proteins*, Science **288**, 7 April 2000, 88–95.
- [29] C. VILLANI *Topics in optimal transportation*, AMS (2003).