Periodically Rocked Thermal Ratchets.

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Abstract. – We consider overdamped Brownian particles in anisotropic, periodic structures (ratchets) that are rocked periodically. Together with the periodic forcing, white thermal noise can generate a non-zero, macroscopic velocity. By tuning the parameters, the direction of the current can be reversed. Additionally, the current as a function of the driving amplitude exhibits several local maxima at finite driving frequencies. For zero thermal noise, the deterministic current assumes an intriguing structure, reflecting the complex dynamics of particle excursions along the ratchet.

Biological applications relating to phenomena such as movement of muscles or the operation of molecular combustion motors involve a transport of Brownian particles along periodic structures in the apparent absence of any external driving forces [1-6]. Hence, the challenge of seeking the physical mechanism(s) of directed transport without having to apply macroscopic bias forces or field gradients has stimulated the interest of many biologists, chemists and physicists (note the series of News and Views contributions in ref. [1]). Indeed, it could be demonstrated theoretically [1-5], as well as experimentally [6], that fluctuation-induced transport is possible in periodic structures with spatial asymmetry (no reflection symmetry). Such systems are termed thermal ratchets. Fluctuation-induced transport requires the presence of non-equilibrium forces $F(t)$: a finite current exists solely due to the fact that the second law of thermodynamics is no longer applicable to these non-equilibrium systems.

In this paper, we study a ratchet-like mesoscopic system, driven by thermal noise and a periodic driving force with zero time average. Since most of the molecular transport occurs in the overdamped regime [2-5], we can safely neglect inertial effects. Much to our own surprise, we find that a periodically driven ratchet exhibits a series of unexpected features, such as the occurrence of current reversal, and a complex, multipeaked current-driving amplitude characteristics.

Starting point of our analysis is the overdamped Langevin equation

$$\dot{x} = -\partial_x \{V(x) - xF(t)\} + \xi(t). \tag{1}$$

The ratchet potential $V(x) = -k^{-1}[\sin(kx) + (1/4)\sin(2kx)]$ has the shape of a sawtooth with smoothed edges (see right-hand side of fig. 2*b*)). In the following we choose $k = 2\pi$, which implies an intrawell relaxation frequency $\omega_0 \approx 3.18$. For the periodic force we take $F(t) = A\sin(\omega t)$. The thermal noise is modelled by a Gaussian white noise $\xi(t)$ with zero mean and the correlation $\langle\xi(t)\xi(t')\rangle = 2D\,\delta(t-t')$. We mention that the spatial average of $\partial_x V(x)$, as well as the time average of $F(t)$ are zero.

It is well known that this stochastic process can be recast in terms of the probability density $W(x, t)$ that satisfies the Fokker-Planck equation $\dot{W}(x,t) = -\partial_x J(x,t)$, with periodic boundary conditions in space. Here

$$J(x,t) = [D^{(1)}(x,t) - D\partial_x]\,W(x,t) \tag{2}$$

is the current density, and $D^{(1)}(x,t) = \cos(kx) + (1/2)\cos(2kx) + A\sin(\omega t)$ is the drift velocity. We are mainly interested in asymptotic averages. Thus we define the average current $\bar{J}$ as

$$\bar{J} = \lim_{t\to\infty} \frac{1}{TL} \int_t^{T+t} \mathrm{d}t' \int_0^L \mathrm{d}x\, J(x,t'), \tag{3}$$

with temporal period $T = 2\pi/\omega$ and spatial period $L = 2\pi/k$. We note that the current in (3) is independent of the initial preparation, because $W(x, t\to\infty)$ assumes a unique limiting periodic distribution in time and space [7, 8]. The result of a unique current holds true even in the limit of zero noise intensity D, because the drift is periodic and different deterministic trajectories do not cross.

To cover an extensive range of parameters, we solved eq. (3) using a matrix continued-fraction method [7, 8], supplemented by analytic results in limiting cases, such as the adiabatic limit.

Figures 1*a*) and *b*) contain our main findings for generic cases: the current $\bar{J}$ is plotted for several driving frequencies ω as a function of the noise strength D and the driving amplitude A. The adiabatic limit $\omega = 0$, drawn as solid lines in fig. 1*a*) and *b*), is readily evaluated

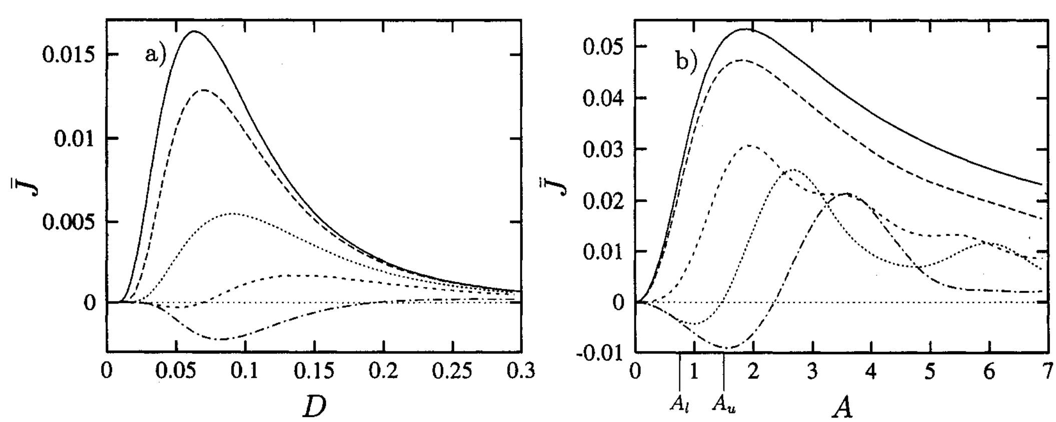

Fig. 1. – *a*) The mean current $\bar{J}$ *vs.* thermal-noise strength D for fixed driving amplitude $A = 0.5$ can change sign. The current for the driving frequencies $\omega = 0.01$, 1, 4, 5.5, and 7 is depicted from top to bottom. The analytic result obtained in the adiabatic limit, eq. (4), coincides with the solid line $\omega = 0.01$. *b*) The mean current $\bar{J}$ *vs.* A for fixed $D = 0.1$ becomes negative for sufficiently high frequencies. The current for the frequencies $\omega = 0.01$, 1, 4, 7, and 10 is depicted from top to bottom. The adiabatic limit falls onto the solid line $\omega = 0.01$.

from the first-order equation (1) yielding

$$\bar{J}_{\mathrm{ad}} = \frac{D}{T}\int_0^T \mathrm{d}t\Big\{[1-\exp[\Phi(L,t)]]^{-1}\cdot \\ \cdot \int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \exp[\Phi(y,t)-\Phi(x,t)] - \int_0^L \mathrm{d}x \int_0^x \mathrm{d}y \exp[\Phi(y,t)-\Phi(x,t)]\Big\}^{-1}, \tag{4}$$

where $\Phi(x,t) = [V(x) - xA\sin(\omega t)]/D$.

First, we observe that the current vanishes asymptotically, both for large A, as well as for large D. This can be understood upon noting that in these limits the influence of the ratchet potential becomes negligible. At $A = 0$ the current vanishes, because here the open system reduces to a system in thermal equilibrium [9]. In the deterministic limit, *i.e.* $D = 0$, the current vanishes identically for all driving amplitudes below a critical threshold A_l (see below), while for $A > A_l$ the current can assume zero or finite values for $D = 0$, depending on ω. Note, however, that for a periodic potential $V(x)$ with reflection symmetry, the average current $\bar{J}$ vanishes identically for any A and D (with $\omega \neq 0$).

More surprising than the facts mentioned up to this point is the result of current reversal in fig. 1*a*), *b*). This characteristic feature seemingly occurs only for driving frequencies which exceed the intrawell relaxation frequency ω_0. In addition one finds several extrema in the current-amplitude characteristics.

To understand these novel features, we first address the deterministic behaviour. In particular it turns out that the intriguing result of a sign change is not exhibited by any deterministic motion! Hence only the mutual interplay between noise and finite-frequency

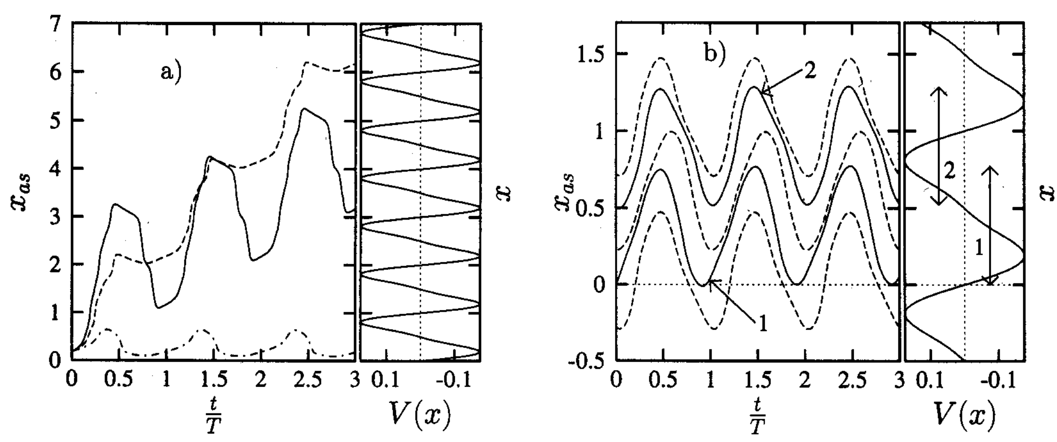

Fig. 2. – *a*) Asymptotic trajectory $x_{\mathrm{as}}(t)$ *vs.* time t for fixed $\omega = 1$. Small driving amplitudes A lead to a periodic motion with zero average current $\bar{J}$: the dash-dotted line shows $A = 1$. For $A = 1.5$ (dashed line), $\bar{J}$ is non-zero; but for $A = 3$ (solid line), $\bar{J}$ is smaller than that of $A = 1.5$. As a guide for the eye, the static potential is included on the right-hand side of the diagram. Note that the system has been started at large negative times t_0 to be in its asymptotic regime at the times $t \geqslant 0$ shown in the figure. *b*) Asymptotic trajectories $x_{\mathrm{as}}(t)$ *vs.* t for fixed $\omega = 7$ and $A = 3$. Note that for this special values of A and ω, there are two distinct stable trajectories (solid lines) that carry no current, and two separatrices (dashed lines). The upper separatrix in the figure is equivalent to the lower one. The arrows within the plot of the potential on the right-hand side show that trajectory 1 is centred around the minimum of the potential, trajectory 2 around the maximum.

driving ($\omega \neq 0$, *i.e.* non-adiabatic) is able to produce this effect. So far we have not been able to find a satisfying (analytical) explanation. We want to point out that the mechanism of this current reversal differs distinctly from that put forward by Doering *et al.* [5], where the sign change of $\bar{J}$ occurs due to a differing *statistics* of non-equilibrium, but stochastic driving forces $F(t)$.

In fig. 2*a*) and *b*) we depict some deterministic, asymptotic trajectories $x_{\text{as}}(t)$. A glance at these trajectories reveals that the deterministic dynamics is indeed a non-trivial problem. First of all, a larger A does not necessarily imply a larger current $\bar{J}$ (fig. 2*a*)). Secondly, for a suitable choice of parameters (here $A = 3$, $\omega = 7$) one can find two distinct stable trajectories (fig. 2*b*)). Hence different initial positions can lie in different basins of attraction for the solution $x(t)$. By looking at the potential on the right side of fig. 2*b*), it can be seen that the path of trajectory 1 is centred around the minimum of the static potential $V(x)$, whereas trajectory 2 explores the region around the potential maximum.

We next go on to consider the average deterministic current. Figures 3*a*) and *b*) show the step-like structure of $\bar{J}$ as a function of the driving amplitude. An important first difference compared to the noise-driven case can be seen immediately: the deterministic current never changes sign. Furthermore, the onset of current occurs at a frequency-dependent threshold value $A_{\min}(\omega)$. Naively one would expect the onset to occur at the amplitude where the tilt of the potential is big enough that the local minima of the ratchet disappear. For the tilt to the right side this happens if $A \geqslant A_{\text{l}} = 0.75$; for the tilt to the left if $A \geqslant A_{\text{u}} = 1.5$. Theoretically and numerically one obtains $A_{\min}(\omega) \geqslant A_{\text{l}}$, with $A_{\min}(\omega \to 0) \to A_{\text{l}}$. In the regime where $\bar{J}$ increases monotonically, the particle can move freely to the right side, but gets trapped in a valley for a tilt to the left side (this mechanism can be termed «mechanical diode»). For $|A\sin(\omega t)| > A_{\text{u}}$, the particle does no longer encounter minima; it, therefore, can move in both directions. This makes a maximum current around $A = A_{\text{u}}$ plausible. Note that, for the adiabatic limit, the current $\bar{J}$ achieves its maximum exactly at $A = A_{\text{u}}$! One obtains the solution of the adiabatic limit for zero noise by integrating eq. (1). The time t a particle needs

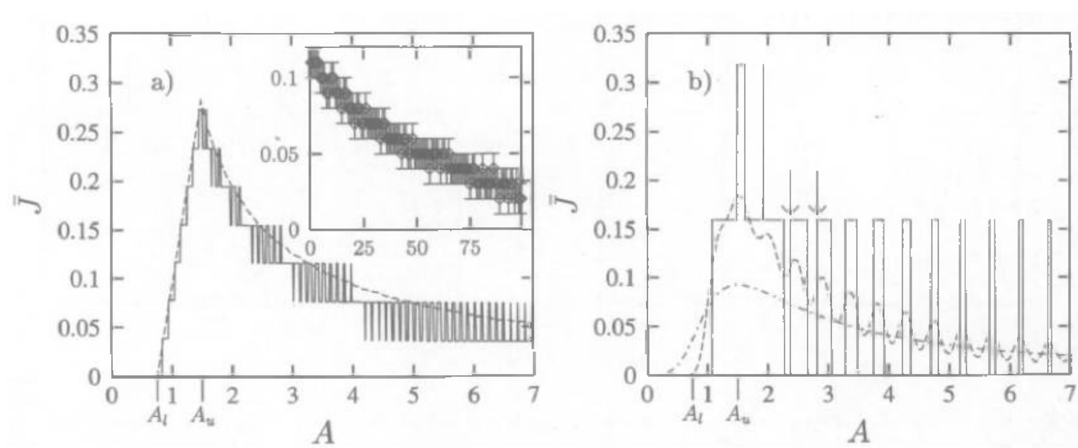

Fig. 3. – *a*) The mean current $\bar{J}$ *vs.* driving amplitude A for zero noise strength $D = 0$ demonstrates how the adiabatic limit is approached. The dashed line is for the frequency $\omega = 0.01$ and falls on top of the adiabatic limit, eq. (6). The solid line depicts the current for $\omega = 0.25$. The current is positive for all driving amplitudes. The adiabatic curve looks smooth, because the height of the steps is proportional to ω (see text). In the inset, the width of the n-th step for $A > 7.8$ is plotted *vs.* n (with error bars). *b*) The mean current $\bar{J}$ *vs.* A for fixed $\omega = 1$ shows the smearing of the deterministic step-like behaviour with increasing noise strength $D = 0$, 0.01, 0.05, from top to bottom. The arrows indicate the «distance» between steps as defined in the text.

to move by a distance of length L equals

$$t(\theta) = \int_0^L dy \frac{1}{D^{(1)}(y, \theta)}, \tag{5}$$

where $D^{(1)}(y, \theta) = \cos(ky) + (1/2)\cos(2ky) + A\sin\theta$. Here, θ is the phase of the slowly varying external force (hence the adiabatic limit). Equation (5) leads immediately to the current for a fixed tilt $A\sin\theta$. A final integration over θ then yields $\bar{J}$:

$$\bar{J} = \frac{1}{2\pi}\int_0^{2\pi} d\theta \frac{L}{t(\theta)}. \tag{6}$$

Adding noise makes the connection to the diagrams 1 above. Finite noise $\xi(t)$ smears the pronounced steps and plateaus of the current curve into a wave-like structure; cf. fig. 3*b*) and fig. 1*b*); we see that the local extrema of fig. 1*b*) are deterministic features—not related to any noise-driving co-operation. Obviously, if the noise strength is increased further, the extrema will eventually disappear, as shown in fig. 3*b*).

Another striking property of the deterministic current is the quantisation of the step height in units of $L\omega/2\pi$, cf. fig. 3. Clearly, in the asymptotic limit, where $\dot{x}_{as}(t)$ is a periodic function of t with periodicity T, the position of the particle at time t differs from the position at time $t+T$ by an integer multiple of L. Put differently, the periodic part of $x_{as}(t)$, namely $x_{as}(t) - \bar{J}\cdot t$, locks onto the phase of the periodic driving [8]. This immediately implies the quantisation. Finally we mention a most peculiar property of the «distance» and width of the steps. Defining the «distance» as being measured from the onset of one step to the onset of the next step (see the two arrows in fig. 3*b*)), our simulations seemingly yield a constant distance between successive steps. Their widths decrease monotonically within constant current $\bar{J}$, as shown in the inset of fig. 3*a*). An exponential function fits the curve satisfactorily, but due to the numerical uncertainty, a definite conclusion cannot be drawn.

To summarize, the overdamped motion of a Brownian particle in an asymmetric potential, driven by a periodic force, exhibits a high degree of complexity, even in the deterministic regime. Mostly by means of numerical calculations we have discovered a number of interesting and unexpected features of this ratchet system. The deterministic ratchet problem is a good starting point for analysing the system in the presence of thermal noise; many features of the latter are an immediate consequence of the deterministic one. But even with the simplest thermal noise, namely Gaussian white noise, a reversal of the current occurs. This feature is neither present in the adiabatic limit (with or without noise), nor in the case of zero noise but finite driving frequency. We therefore conclude that it is caused by a co-operative interplay between noise and deterministic, finite-frequency driving.

It should be noted that our «rocking ratchet» device may also have a variety of important applications in nano-technology. For example, it can be utilized to efficiently separate particles with nearly equal diffusion coefficient due to the Arrhenius-like sensitivity of the current *vs.* diffusion strength (cf. the behaviour of $\bar{J}$ in fig. 1*a*) at small D).

There are a number of further studies suggested by the results presented here: the novel phenomena we have observed for periodically driven ratchets are expected to be robust under incoherent forcing, such as a stochastic, non-equilibrium harmonic-oscillator process $F(t)$ (harmonic noise [10]). Additionally, the intriguing deterministic features of eq. (1) are expected to stimulate future theoretical work on non-autonomous differential equations [11] that are periodic both in space and time.

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