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STATISTICAL DISTRIBUTIONS FOR HAMILTONIAN SYSTEMS COUPLED TO ENERGY RESERVOIRS AND APPLICATIONS TO MOLECULAR ENERGY CONVERSION*

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We study systems with Hamiltonian dynamics type coupled to reservoirs providing free energy which may be converted into acceleration. In the first part we introduce general concepts, like canonical dissipative systems and find exact solutions of associated Fokker–Planck equations that describe time evolutions of systems at hand. Next we analyze dynamics in ratchets with energy support which might be treated by perturbation theory around canonical dissipative systems. Finally we discuss possible applications of these ratchet systems to model the mechanism of biological energy conversion and molecular motors.

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1. Introduction

The study of mechanical systems with support of energy goes back to the investigations of Helmholtz and Rayleigh on the origin of sustained oscillations. In his fundamental book "The theory of sound", published 1894, Rayleigh proposed the following equation as the basis for the treatment of sustained oscillations

$$\frac{dv}{dt} + \omega_0^2 x = (a - bv^2)v\,. \tag{1}$$

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Here x, v are the position and velocity of the oscillator of a mass $m = 1$, ω_0 its frequency and a, b are positive constants which determine the input of energy according to the balance for the Hamiltonian H:

$$\frac{dH}{dt} = (a - bv^2)v^2 \,. \tag{2}$$

We see from (2) that for small velocities the energy input (and correspondingly the acceleration of the particle) is positive up to the state, when the velocity reaches the characteristic value $v_0 = \pm\sqrt{a/b}$. Generalizations of the "active friction" introduced by Rayleigh found many applications including the concept of "Active Brownian Motion" which extends the notion of standard Brownian motion as studied by Einstein, Smoluchwski, Fokker, Planck and others to the field of driven motions [1–5, 9] including a developing theory of swarming motions [6–8, 10, 11]. In the second section we introduce the concept of canonical-dissipative systems, which was developed by Haken and Graham [12, 13], and proved to be very useful in the context of systems with energy support [2, 14, 15].

In the remaining part of the paper we study more specific applications to transport problems on Hamiltonian ratchets, to molecular energy conversion and to molecular motors. Since the fundamental work of Smoluchowski [16] the problem of transport on ratchets is under a constant debate. Some of the most interesting applications are related to biological energy conversion [17, 18]. Here we will discuss several problems related to Hamiltonian ratchets and their possible role in modeling the functioning of ATP and ADP in cells and the related transport mechanisms. We have in mind possible applications to biological systems as *e.g.* proton and electron pumps. In particular we are interested in the role of the ATP-synthese. One of the aims of our work is to explore the possibility to model the absorption of ATP as an energetic support from an energy reservoir. The basic model assumption is that free energy is provided by an ATP reservoir in continuous or discrete form and transferred into a ratchet. The energy quanta formed by hydrolysis of ATP are able (in principle) to provide work and move the particle "uphill". This could imply a movement of the particle against a mechanical or electrical potential gradient. We propose two schemas how to transform the ATP-energy into work:

(i) by a continuous support with free energy which is converted to work, or

(ii) by absorption of energetic quanta which are modeled as a kind of energetic shot noise.

2. Canonical-dissipative dynamics as a solvable case of driven systems

The Rayleigh equation cannot be solved exactly in an analytic form. However with a little change in the driving term we can get a solvable problem. For the motion on a limit cycle of radius r, dynamic equilibrium conditions between centripetal and centrifugal forces require

$$\begin{aligned} \frac{mv^2}{r} &= m\omega^2 r\,, \\ E &= mv^2\,, \end{aligned} \tag{3}$$

so that, due to the equipartition of energy the relation

$$\langle v^2 \rangle = \frac{\langle H \rangle}{m} \tag{4}$$

holds. This may justify to make in Eq. (1) the replacement

$$v^2 \to \frac{H}{m}\,, \tag{5}$$

which for linear oscillators is not true at any time moment, but holds in average. By the replacement (5) we get a system which is solvable as was observed already by Poincaré

$$m\left(\frac{dv}{dt} + \omega_0^2 x\right) = \left(a - \frac{b}{m}H\right)v\,. \tag{6}$$

Since

$$H = \frac{mv_0^2}{2} + \frac{m\omega_0^2 x^2}{2} = H_0 = m\frac{a}{b} \tag{7}$$

is an invariant and an attractor of Eq. (6), all trajectories converge to the surface $H = H_0$. The motion on this surface is purely Hamiltonian in nature and the solution is the standard one of a linear oscillator with just this energy. The exact solution of the dynamic equations on the surface $H = H_0$ is

$$x(t) = \left(\frac{v_0}{\omega_0}\right)\sin(\omega_0 t + \delta)\,, \qquad v(t) = v_0 \cos(\omega_0 t + \delta)\,. \tag{8}$$

This stable motion corresponds to a sustained oscillation with stationary amplitude $x_0 = v_0/\omega_0$ which represented in the phase space form a closed separated orbit, *i.e.* a limit cycle. Systems of this type, characterized by dissipative forces depending only on the form of Hamiltonian were called later by Graham "canonical dissipative" [13]. The stochastic theory of this rather interesting class of systems was developed by Klimontovich [1] starting with a Langevin analogue of Eq. (6) that incorporates action of random (white and Gaussian) forces $\xi(t)$:

$$m\left(\frac{dv}{dt}+\omega_0^2 x\right)=\left(a-\frac{b}{m}H\right)v+m(2D_v)^{1/2}\xi(t)\,, \tag{9}$$

with D_v representing strength of velocity fluctuations. The full (2-dimensional) Fokker–Planck equation corresponding to Eq. (9) reads ($m=1$)

$$\frac{\partial P(x,v,t)}{\partial t}+[H,P]=\frac{\partial}{\partial v}\left[(bH-a)\,vP(v,t)+D_v\,\frac{\partial P(v,t)}{\partial v}\right] \tag{10}$$

with the RHS representative for the dissipative motion. This equation has the stationary solution which factorizes to the product of functions (in x and v variable, respectively) with the stationary probability density $P_0(v)$ given by

$$P_0(v)=\rho(H)=C\exp\left[\frac{aH-bH^2/2}{D_v}\right]. \tag{11}$$

For the passive case, $a<0$, this distribution is quite similar to a Maxwellian. For $a>0$ the system is driven away from equilibrium. In this case the velocity distribution is bistable and has a maximum above the limit cycle

$$\frac{v^2}{2}+\frac{\omega_0^2 x^2}{2}=\frac{a}{b}\,. \tag{12}$$

This corresponds to a system of particles which perform self-sustained oscillations. For $a<0$ the oscillations are damped, for $a=0$ the deterministic system goes through a bifurcation which leads for $a>0$ to the auto-oscillating regime. The distribution function for the transition point has a rather large dispersion as characteristic for all phase transitions. In the limit of small noise ($D_v\to 0$) the curve of maximal probability is exactly above the deterministic limit cycle. This is, of course, a necessary condition which any correct solution of the Fokker–Planck equation has to fulfill. Further we note, that the term in the exponent $(H-a/b)^2$ corresponds to the Lyapunov function of the system. We found this way a model system which is exactly solvable in equilibrium and for any distance away from equilibrium. Admittedly, the force function which we used, $F=(a-bH)v$ is not very realistic. However it may be shown, that the more realistic Rayleigh force $F=(a-bv^2)v$ introduced for modeling sound oscillations as well as the van der Pol force $F=(a-bx^2)$ introduced for modeling electric oscillations may be converted in good approximation to our canonical-dissipative force $F = (a - bH)v$. This may be proven by using the procedure of phase-averaging [1]. Our solvable model system is quite useful as a starting point for perturbative schemes. Now we will generalize the concept and treat a whole class of solvable systems. This idea is mainly based on works of Haken and Graham [12, 13]: For this special class of far from equilibrium systems, a general ensemble theory similar to Gibbs approach may be developed [12–14]. The theory of canonical-dissipative systems is the result of an extension of the statistical physics of Hamiltonian systems to a special type of dissipative systems where conservative and dissipative elements of the dynamics are both determined only by invariants of the mechanical motion. There exists close relation to a recently developed theory of active Brownian particles [3, 15]. We start the development of the theory of canonical-dissipative systems with a study of the phase space dynamics of a driven many-particle system with f degrees of freedom $i = 1, ..., f$. Assuming that the Hamiltonian is given by $H(q_1...q_f p_1...p_f)$ the mechanical motion is given by Hamilton equations. The solutions are trajectories on the plane $H = E =$const. The constant energy $E = H(t = 0)$ is given by the initial conditions, which are (in certain limits) arbitrary. We construct now a canonical-dissipative system with the same Hamiltonian

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} - g(H)\frac{\partial H}{\partial p_i}\,, \tag{13}$$

assuming that the dissipation function $g(H)$ is nondecreasing. Equation (13) defines a canonical-dissipative system which does not conserve the energy. In regions of the phase space where $g(H)$ is positive, the energy decays and in regions where $g(H)$ is negative, the energy increases. The simplest possibility is constant friction $g(H) = \gamma_0 > 0$ which corresponds to a decay of the energy to the ground state. Of more interest is the case when the dissipative function has a root $g(E_0) = 0$ at a given energy E_0 *e.g.*

$$g(H) = c(H - E_0)\,. \tag{14}$$

Then the states with $H < E_0$ are supported with energy, and from states with $H > E_0$ energy is extracted. Therefore, any given initial state with $H(0) < E_0$ will increase its energy up to reaching the shell $H(t) = E_0$ and any given initial state with $H(0) > E_0$ will decrease its energy up to the moment when the shell $H(t) = E_0$ is reached. The surface $H = E_0$ is an attractor of the dynamics, any solution of Eq. (13) converges to it. On the surface $H = E_0$ itself the solution corresponds to a solution of the original Hamiltonian equations for $H = E_0$. The speed of the relaxation process is proportional to c^{-1}. More general dissipative functions were considered in the theory of active Brownian motions [15]. We mention that in particular all noninteracting systems are canonical-dissipative. The attractor of the dissipative system (13) is located on the surface $H = E_0$. This does not mean that the full $(2f-1)$-dimensional surface is the attractor of the system. Such a statement is correct only for the case $f = 1$, which has been considered in the last section, further this statement may be true also for systems which are ergodic on the surface $H = E_0$. In the general case the attractor may be any subset of lower dimension, possibly even a fractal structure.

A more general class of canonical-dissipative systems is obtained, if beside the Hamiltonian also other invariants of motion are introduced into the driving functions. Let us assume that the driving functions depend on $H = I_0$ and also on some other invariants of motion $I_0, I_1, I_2, ..., I_s$. For the equation of motion we postulate

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} - \frac{\partial G(I_0, I_1, I_2, ...)}{\partial p_i} \,. \tag{15}$$

These are generalized canonical-dissipative systems.

We return to the simpler case $g = g(H)$ and include an external white noise source which leads us to the Langevin equations

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} - g(H)\frac{\partial H}{\partial p_i} + (2D(H))^{1/2}\xi(t)\,. \tag{16}$$

The essential assumption is, that noise and dissipation depend only on H. The corresponding Fokker–Planck equation reads

$$\frac{\partial \rho}{\partial t} + \sum \frac{\partial H}{\partial p_i}\frac{\partial \rho}{\partial q_i} - \sum \frac{\partial H}{\partial q_i}\frac{\partial \rho}{\partial p_i} = \sum \frac{\partial}{\partial p_i}\left[g(H)\frac{\partial H}{\partial p_i}\rho + D(H)\frac{\partial \rho}{\partial p_i}\right]. \tag{17}$$

An exact stationary solution is

$$\rho_0(q_1...q_f p_1...p_f) = Q^{-1}\exp\left(-\int_0^H dH'\,\frac{g(H')}{D(H')}\right)\,. \tag{18}$$

The derivative of ρ_0 vanishes if $g(H = E_0) = 0$. This means, the probability is maximal at the surface $H = E_0$. For the special case of a linear dissipation function we find the stationary solution

$$\begin{aligned}\rho_0(q_1...q_f p_1...p_f) &= Q^{-1}\exp\left(\frac{cH(2E_0 - H)}{2D}\right) \\ &= Q_1^{-1}\exp\left(\frac{-c(H - E_0)^2}{2D}\right)\,. \end{aligned} \tag{19}$$

Although these distributions might be formally correct they, nevertheless, may be not of interest for applications to problems of physics. In particular, distributions of type (18) do not admit translational or rotational flows. In order to include such properties, other invariants of motion may be introduced [2] or perturbations which break the high symmetry of the canonical-dissipative systems.

The rest of the paper is devoted to applications of the concept of canonical-dissipative systems to ratchet systems. We will show that canonical-dissipative systems are a useful concept which allows to treat these systems on the basis of perturbation theories. We will study ratchets coupled to energy reservoirs and possible applications to molecular energy conversion and special types of molecular motors.

3. Hamiltonian ratchets coupled to sources of energy

3.1. Models of the ratchet and the energy source

In recent papers several new types of inertia ratchets with energy input were studied which are related to our problem of canonical-dissipative systems [22, 23]. Let us consider first a 1D-ratchet system described by the Hamiltonian $H = p^2/(2m) + U(x)$, consisting of a particle located at x with momentum $p = mv$, subjected to the action of a periodic potential.

As a particular simple case we consider the continuous ratchet potential introduced by Mateos, Machura and others [24, 25]. This potential model $U(x)$ has one free parameter (h, the height of the maximum)

$$U(x) = h\{0.499 - 0.453\{\sin[2\pi(x+0.1903)] + 0.25\sin[4\pi(x+0.1903)]\}\}\,. \quad (20)$$

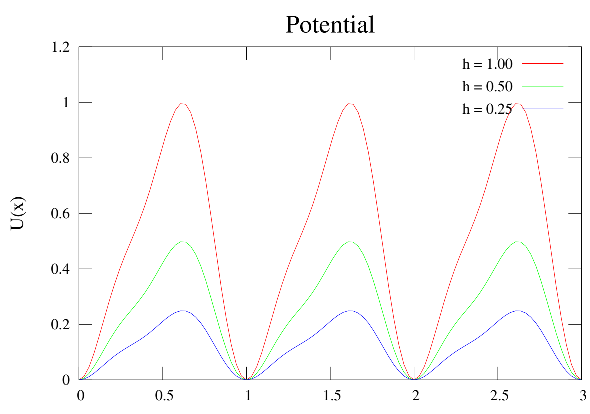

Fig. 1. Ratchet potentials of the type proposed by Mateos *et al.* [24, 25] with different height $h = 1.0, 0.5, 0.25$.

Finally, we use for comparison also the quasilinear (continuous but not differentiable) standard ratchet which is in the first segment defined by [22]

$$U(x) = -F_1 x \,, \qquad \text{if} \quad 0 < x < x_\mathrm{m} \,, \tag{21}$$

$$U(x) = -F_2(x-1) \,, \qquad \text{if} \quad x_\mathrm{m} < x < 1 \,, \tag{22}$$

where

$$F_1 = -\frac{h}{x_\mathrm{m}} \,, \qquad F_2 = \frac{h}{1-x_\mathrm{m}} \,. \tag{23}$$

Here $0 < x_\mathrm{m} < 1$ is the place of the maximum. The ratchet potentials introduced above have all the period 1. We assume that the basic cell of periodic boundary conditions is $L = 1$ or $L > 1$ (integer). It is important to realize that the excitations might have a period which is larger than the period of the basic cell. Having in mind biological applications where typically some transfer from chemical to mechanic or electric energy appears, we will study now ratchets which are connected to an energy reservoir. The driving force is in our model proportional to the velocity and has a time dependence defined by an extra equation for a depot energy $e(t)$:

$$\frac{dv(t)}{dt} + \gamma v(t) + U'(x) = F_0 + de(t)v(t) + \sqrt{2D}\xi(t) \,, \tag{24}$$

$$\frac{de(t)}{dt} = q(t) - ce(t) - de(t)v^2(t) \,. \tag{25}$$

Here γ is a mechanical friction, $q(t)$ may be a deterministic or stochastic source of energy, d is a transmission rate and F_0 stands for a possible tilt of the ratchet. The mass m has been set to $m = 1$. The physical meaning is that we have a permanent inflow of energy, which in simplest case is constant $q(t) = q_0 =$const., and flows with rate $dv^2(t)e(t)$ to the mechanical degree of freedom. The term $ce(t)$ expresses the rate of internal losses in the depot. The driving mechanism corresponding to Eq. (25) is a generalization of the Rayleigh system discussed above [3, 4, 22, 23]. We use here a mechanical interpretation but due to the equivalence of mechanical and electrical circuits, it could as well be an electrical circuit which is modeled by our equations. There exist other driving mechanisms which are nearer to the van der Pol oscillator, but we leave a study of these mechanisms to future work.

3.2. The cases of free particles and constant external force

We will solve now the deterministic equations for several instructive special cases:

$$\ddot{x}(t) + U'(x) + [\gamma - de(t)]\dot{x}(t) = F_0 \,, \tag{26}$$

$$\dot{e}(t) - q + ce(t) + de(t)\dot{x}^2(t) = 0 \,. \tag{27}$$

As a zeroth approximation we neglect in the first equation the potential assuming $U'(x) = 0$ and assume stationarity *i.e.* $\dot{e} = 0$. This leads to the case of *free motion* ($U(x) =$ const). Treating the set of equations we make use of the equilibrium relation for the first equation $e = d/\gamma$ which is due to the stable flux of energy that counterbalances the dissipation term. We will take later this exact solution as the starting point of a perturbation theory. The bifurcation parameter of our problem is

$$\beta = \frac{q}{\gamma} - \frac{c}{d}\,. \tag{28}$$

If $\beta \geq 0$, the system is driven to non-equilibrium states and has all together 3 stationary states of the velocity: $v = 0$, $v = v_0$ and $v = -v_0$. Here v_0 is the velocity where friction and stationary driving compensate each other. The state $v = 0$ is unstable. The condition of equilibrium leads to

$$e_0 = \frac{q}{c + dv_0^2} \Rightarrow v_0^2 = \frac{q}{\gamma} - \frac{c}{d}\,. \tag{29}$$

For small energy transfer, such as for low amplitude of the corresponding limited dynamics, the particle gets trapped in one well and does sustained oscillations similar as described by the original. The case of trapped motions is not studied here, we refer to another paper [26].

We consider now the case of a constant force, corresponding to a constant tilt

$$F = F_0 = -a\,. \tag{30}$$

Here a is the slope of an equivalent potential $U_0(x) = -ax$. Mostly we will assume a positive slope $a > 0, F_0 < 0$. Let us first consider the case that there is no additional ratchet potential *i.e.* $U(x) = 0$. This problem still admits an exact solution. Without an energy flux q from the reservoir, the particle would fall down (if $a > 0$ from right to left). Including the reservoir provides the possibility of uphill motions. The condition of stationary motion under the action of this force leads to the cubic equation

$$\gamma d v_0^3 + a d v_0^2 + (c\gamma - qd) v_0 + ac = 0\,. \tag{31}$$

The solutions may be found graphically (see Fig. 2) Somehow simpler is the solution in the case $c = 0$, *i.e.* there is no internal dissipation. Then we get the explicite solution

$$v_0 = -\frac{a}{2\gamma} \pm \sqrt{\frac{a^2}{4\gamma^2} + \frac{q}{\gamma}}\,. \tag{32}$$

In this limit the solution is bistable and does not depend on the parameter d. We may improve this result if we assume that dissipation c and the slope a are so small that ac may be neglected. This leads to the solution

$$v_0 = \frac{F_0}{2\gamma} \pm \sqrt{\frac{F_0^2}{4\gamma^2} + \frac{q}{\gamma} - \frac{c}{d}}\,, \tag{33}$$

This way, in the general case we have a cubic equation for the stationary velocities, which is easy to solve numerically, and in some approximation analytically. The downhill motion exists in all cases, for our standard case $a > 0; F_0 < 0$ the downhill motion is directed to the left. However, in the case of positive energy input $q_0 > 0$ also a stationary uphill motion may exist $v_0 > 0$, provided the force driving downhill is not too large. For example if $a = 1; F_0 = -1$, the trivial downhill solution is $v_0 = -5$ and the stable uphill solution is $v_0 = +0.5$ for $d = 1$; for $d = 0.3$ no uphill solution exists. It is interesting to note that uphill motion may exist even without any ratchet effects provided the driving is sufficiently strong. However, even if uphill motion is possible, the question remains, what is the influence of ratchet effects and what is the efficiency of the energy transfer.

The results which we obtained for constant forces allow us a simple approximation of the dynamics for the piecewise linear potentials defined by Eq. (22). These ratchets are formed of two segments each with constant force. The first one is increasing with $a_1 = h/x_{\rm m} > 0$ and the second one

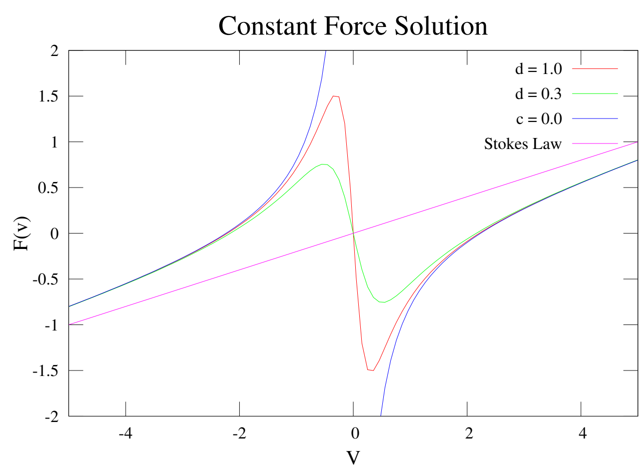

Fig. 2. Stationary solution: The force $F_0 = -a$ as a function of the velocity for $\gamma = 0.2$ and 2 fixed d-values ($d = 0.3$ and $d = 1$ with $c = 0.1$) and the asymptotic curve with $c = 0$. The comparison is made with Stokes law $F = \gamma v$. The solution representing free motion corresponds to the roots on the axis $F = 0$.

is decreasing with $a_2 = h/(x_{\rm m} - 1) < 0$. In a rough approximation we may compose the dynamics from two pieces corresponding to constant force dynamics, the approximative character is due to the fact that the segments have a finite length, while the solutions given above assume strictly speaking infinite length.

In our approximation we see the conditions for ratchets with unidirectional current:

(i) The average value of the flatter slope should be in the range where the uphill motion is possible, and

(ii) the average value of the steeper slope should not allow the uphill motion.

Under these conditions the particle can go uphill from left to right, however the motion backwards is not possible and we get a unidirectional motion. We may take this construction as a rule of thumb in order to to find the conditions for constructing unidirectional ratcheting devices.

4. The flux regime of ratchets coupled to energy reservoirs

4.1. Analytical results and simulations

In the general case, the equations of motion for ratchets coupled to energy reservoirs cannot be solved analytically. However a few analytical results may be obtained by using perturbation expansions around the solvable cases, which are in fact canonical-dissipative systems. As pointed out above, for small energy input the particle cannot leave a well, its getting trapped and possibly even comes to rest at the bottom. Accordingly we have 3 regimes:

(i) complete rest (point attractor of the dynamics),

(ii) sustained oscillations in one well (bounded attractor),

(iii) flux regime (open attractors).

We leave a detailed investigation of the different regimes to another work [26] and study here only the flux regime which is most interesting for applications.

In the framework of perturbation theory we write

$$v = v_0 + v_1(t) + \dots\,, \qquad e = e_0 + e_1(t) + \dots\ , \tag{34}$$

where v_0, e_0 represent the exact solutions for free motion given above. For large driving and small forces ($U'(x) \approx 0$) the particles move nearly free. We find for free motion two attractors of the velocity

$$v_0^+ = \sqrt{\beta}\,, \qquad v_0^- = -\sqrt{\beta}\,, \qquad e_0 = \frac{\gamma}{d}\,. \tag{35}$$

We take these solutions as the first term in a perturbation series. Inserting the *zero*-approximation into the Eq. (26), with an appropriate choice of the constant the first order of approximation is:

$$v_1(x) \approx v_0 - \frac{U(x)}{v_0} + \frac{h}{2v_0}\,. \tag{36}$$

The solutions given here may be further developed [26]. The perturbation theories are limited in range of validity to ratchets with small height h, *i.e.* ratchets with a rather flat profile. In the opposite case of a strong profiles we may get some good estimates form the formulae for constant tilt, assuming that the motion consists of two parts, the uphill and the downhill motion, which both are described by our formulae for constant force.

In general however, one is forced to rely on simulations. We have carried out a few simulations for ratchets with parameters of interest for the problem of transformation energy input to work. Already Tilch *et al.* [22] have shown by simulations for the case of ratchets with piecewise constant forces, that around the stationary states v_0^+ and v_0^- the dynamical system possesses — at least for larger values of driving — open attractors corresponding to left or right current states [22]. In the present work we have studied several realizations of systems driven in Mateos ratchets potential. As we see in Fig. 3 the Mateos ratchet driven by active friction with strong coupling depot-particle (strong energy transfer *i.e.* strong driving) also possesses several kinds of momentum-dependent attractors: Closed attractors

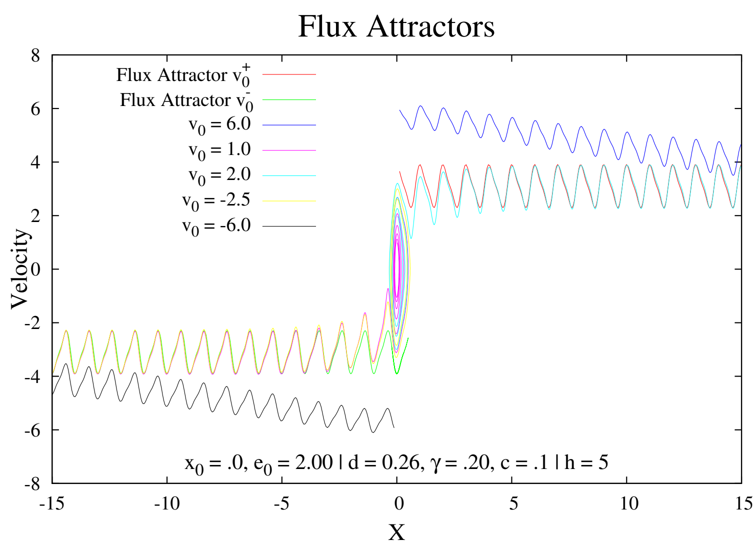

Fig. 3. Examples for trajectories which go to different attractors starting from different initial velocities. Due to the ratchet asymmetry negative initial velocities can give rise to positive asymptotic ones and *vice versa*.

corresponding to limit cycle oscillations on one of the wells, and open attractors. Fig. 3 shows for different initial velocities ($v(0) = 6; 2; 1; -6$), that depending on the initial conditions either one of the open attractors (left or right driven translation) or a closed attractor (sustained oscillation in one particular well) is approached. Another example is shown in Fig. 4. Here we investigated a rather steep continuous Mateos ratchet with $h = 7$. We see in the upper part of Fig. 4 the shape of the ratchet and in the lower part an open right left trajectory in intermittence with a transient limit cycle.

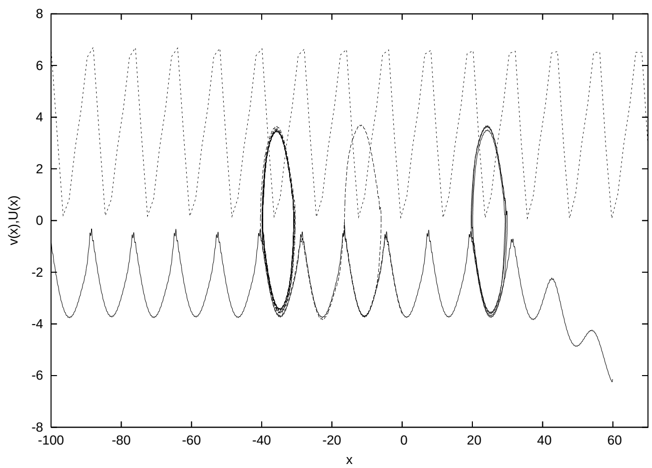

Fig. 4. Simulation results for a very steep Mateos ratchet $h = 7$ which is shown above. The parameters of driving are $q = 1, c = 0.1, d = 1.2$. Two trajectories are shown, the first one makes a transient limit cycle and then is running to the left. A second trajectory starting from a different initial condition is trapped first in a transient cycle and then in a stable limit cycle.

4.2. Tilted ratchets

Under the name *tilted ratchets* we understand here ratchets with a constant average slope. In other words we have a global incline of the ratchet which is due to some constant average force. This may model a constant external load against which the ratchet has to do work. In our example we studied a tiltet ratchet with $h = 0.5$ and a load force which is directed right to left, the force parameter is $a = 0.03$. The parameters of driving are as before $q = 1, c = 0.1, \gamma = 0.1$. As demonstrated in Fig. 5 the attractor of the uphill motion has a big attractor region which is trapping most initial conditions even such with (small) negative initial velocity. However, if the initial velocity is negative and large enough, the trajectory will be trapped by the downhill attractor.

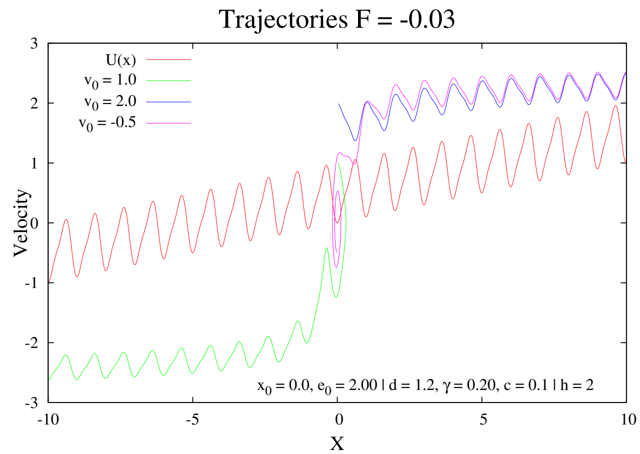

Fig. 5. Examples of uphill flux on a tiltet ratchet with $h = 0.5$. The load force is directed right to left, the force parameter is $a = 0.03$. The attractor of the uphill motion has a big attractor region. However, trajectories with a large negative initial velocity as shown below, may be trapped by the downhill attractor.

The ratchet system which we studied above is in principle able to perform work on the cost of chemical energy imported by the flow $q > 0$. However, it is not excluded that large (negative) fluctuations will bring the system to the downhill attractor. Therefore, we were looking for conditions were only the uphill attractor exists. Studying Mateos ratchet we made a choice of parameters such that the average of the smaller slope (increasing left to right) can still be overcome by the driving mechanism. However, the large slope (from right to left) is too large to be overcome. In other words, there exists an uphill solution for the smaller slope and no uphill solution for the larger slope. This prevents any possibility to go left in our case. The ratchet with such parameters is a unipolar, rectyfying device.

5. The influence of noise

5.1. Langevin white noise in the mechanical equations

In the simplest case we have only Langevin white noise modeling a stochastic uncorrelated force acting on the particle of unit mass $m = 1$

$$\frac{dv(t)}{dt} + \gamma v(t) + U'(x) = F_0 + de(t)v(t) + \sqrt{2D}\xi(t)\,, \tag{37}$$

$$\frac{de(t)}{dt} = q - ce(t) - de(t)v^2(t)\,, \tag{38}$$

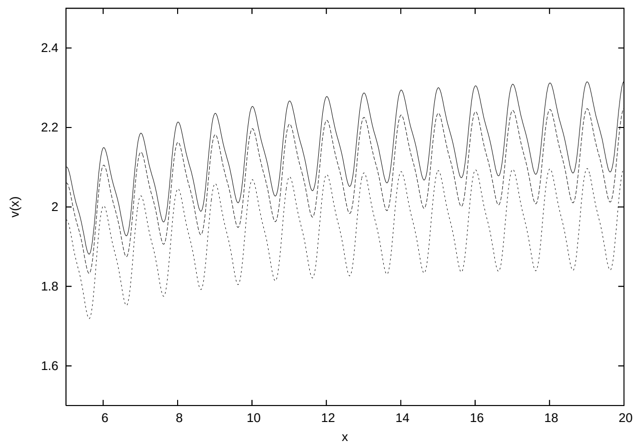

Fig. 6. Example of an unidirectional flux in a Mateos ratchet with $h = 0.2$ and the driving parameters $q = 1, c = 0.1, d = 1$ for a series of tilts with increasing loads $a = 0, 0.03, 0.1$. With increasing load the velocity decreases, however downhill motion is impossible.

where q is the constant source of energy. In the stationary case ($\dot{e} = 0$) and neglecting the energy fluctuations in the reservoir the Fokker–Planck equation reads

$$v\frac{\partial P(x,v)}{\partial x}+F(x)\frac{\partial P(x,v)}{\partial v}=\frac{\partial}{\partial v}\left[\left(\gamma-\frac{qd}{c+dv^2}\right)vP(x,v)+D\frac{\partial P(x,v)}{\partial v}\right].\quad(39)$$

In the case of $U'(x) = F_0 = 0$ the corresponding Fokker–Planck equation may be solved exactly. The solution reads [5]

$$P_0(v) = C\exp\left[-\frac{\gamma v^2}{2D} + \frac{q}{2D}\log\left(1 + \frac{d}{c}v^2\right)\right]. \quad (40)$$

Including a coordinate-dependent force expressing the tilt and a ratchet force $F(x) = -a - U'(x)$ the Fokker–Planck equation may be solved by perturbation theory. In the special case of constant force $F = -a$ we get ($m = 1$)

$$P_0(v) = C\exp\left[-\frac{\gamma v^2 + 2av}{2D} + \frac{q}{2D}\log\left(1 + \frac{d}{c}v^2\right)\right]. \quad (41)$$

This solution gives now an unsymmetrical distribution with two maxima corresponding to the deterministic stable flux velocities (see Fig. 7).

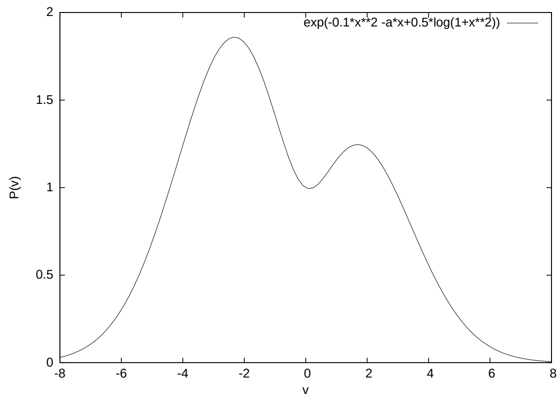

Fig. 7. Example of an unsymmetrical velocity distribution corresponding to a flux on the tiltet ratchet. The downhill motion has a higher probability.

The stochastic flux on a ratchet may be estimated from the formula

$$J = \int dvvP(x,v)\,. \tag{42}$$

Another useful quantity is the fraction of particles with positive or negative net velocity in average over a larger time. We started an experiment with the initial condition

$$P(x,v,t=0) = \delta(x)\delta(v) \tag{43}$$

and measured after some time $T \simeq 300$ the fraction of particles which are located in the positive half-space.

$$\frac{N_r}{N} = \int_0^\infty dx \int dvP(x,v,T)\,. \tag{44}$$

This quantity shows, how strong might be the influence of thermal noise on the transport on ratchets. Fig. 8 displays an example of the fraction of the right-going particles as a function of the noise strength and for different values of the tilt. The non-monotonous character of that partition is surprising and calls for some further explanations of the dynamics.

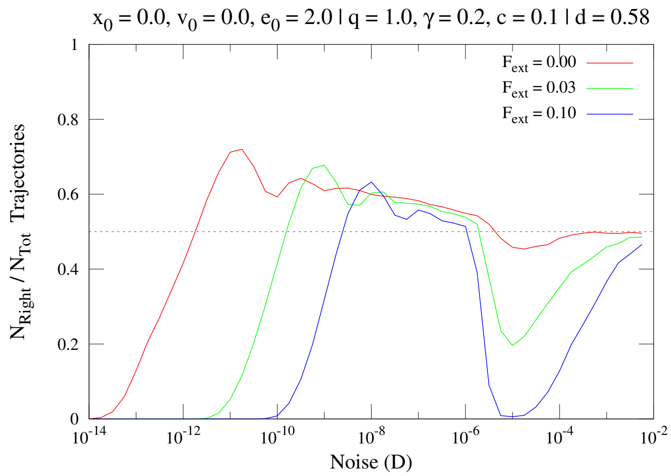

Fig. 8. Example of noise influence on the fraction of particles moving right in average over a time $T \simeq 300$ in dependence on the noise strength for different tilts.

5.2. Shot noise in the energy dynamics

In this model we will assume that the energy input $q(t)$ consists of quanta all of the same energy δe which arrive at stochastic times which are Poisson-distributed.

$$\frac{de(t)}{dt} = q(t) - ce(t) - de(t)v^2(t)\,. \tag{45}$$

The idea is, to model processes similar to the ATP absorption. In ATP-driven processes the system absorbs energy in packets (quanta), each of about $13\,k_{\mathrm{B}}T$. The ATP quanta have nearly the same intensity $\delta e \simeq (1/3)\,\mathrm{eV}$ and are assumed to be independent events whose occurrence in a given time-interval follows a uniform (in time) Poisson process. In such case the time-distance between subsequent events (the waiting time distribution) of absorbtion is stochastically distributed and can be well approximated by an exponential distribution. In the simplest possible case with no energy transfer to the ratchet system $d = 0$, the energy of the reservoir evolves in time following the pattern of an Ornstein–Uhlenbeck process driven by a shot noise:

$$\frac{de(t)}{dt} = -ce(t) + q(t)\,. \tag{46}$$

Shot noise and corresponding applications have been carefully explored since the pioneering works of Campbell (1909) and Schottky (1918). For newer investigations and analysis of the asymptotics to the process Eq. (46), we refer to [27–29]. Obviously, the situation, as described in our model is by far more complicated, since the additional coupling between the energy source and mechanical degrees of freedom does not allow to analyze both equations separately. Staring with this remark, we shall investigate only a few features of our model, leaving a more detailed study to a future work [31]. In a decoupled limit, the energy balance Eq. (45) leads to the following deterministic equation for the means

$$\frac{d\langle e(t)\rangle}{dt} = \langle q(t)\rangle - c\langle e(t)\rangle - d\langle e(t)\rangle\langle v^2(t)\rangle \tag{47}$$

and in the stationary state to

$$\langle e\rangle = \frac{\langle q(t)\rangle}{c + d\langle v^2\rangle}\,. \tag{48}$$

If the shot noise is sufficiently dense in time and the intensity of distributed energy quanta is high enough, we may expect the same behavior as with a continuous energy support. In other words, replacing $\langle q(t)\rangle$ by a constant (or slowly varying function q_{eff}) yields qualitatively the same results as described in former paragraphs.

In contrast, if the distributed energy quanta are small, a new class of phenomena may be expected. During a shot the energy reservoir is filled with one energy portion which has to be consumed in the time interval up to the next shot. In an extreme case the scenario is the following:

(i) At some time the reservoir is empty, the system waits in a minimum of the ratchet-type potential for the energy support.

(ii) After some (exponentially-distributed) stochastic time one energy quantum δe is absorbed.

(iii) Using the given quantum, the particle may move up the next of the neighboring hills, up to the moment when the reservoir is empty again.

Then the particle comes to rest and the cycle may begin again with step *(i)*. There exist several possibilities to model shot noise. We study here only white shot noise (WSN) consisting of a sum of delta-functions [30]. We tested a white shot noise with a number of spikes Poissonian distributed in time and, consequently, with the waiting times distributed according to

$$P(\delta t) = \frac{1}{\tau_c}\exp\left(-\frac{\delta t}{\tau_c}\right)\,, \tag{49}$$

where $\tau_c = \langle\delta t\rangle$ and quanta per shot $Q = 3$. We have performed several test simulations of the process driven by a Poisson shot-noise. Our experience is that driving by a Poisson noise whose variance is equal the mean is inefficient for processes undergoing motion in steep ratchets. For this reason, we first examined motion in a rather flat Mateos' ratchet-potential with $h = 1$. For illustration we display an exemplary result in Fig. 9, in comparison to the case of constant energy influx. The parameter of a constant energy influx was adapted in such a way that in both cases the average energy content of the reservoir is the same. The Mateos ratchet used for the simulations demonstrated in Fig. 9 is rather flat $h = 1$ compared to earlier examples. The motion is driven by a Poisson-type shot noise with the characteristic time $\tau_c = 0.1$ and quanta $Q = 3$. We show for comparison the results for a ratchet driven by a constant energy input $q = 1.2$. The apparent variations in the energy content, as displayed in the right corner of Fig. (9) are due to the Poisson distribution of energy spikes. In the two upper panels the velocity and the coordinate as functions of time are presented. The left corner panel below displays in turn, the velocity as a function of space. The parameters are chosen in such a way that the energy content of the reservoir is in average equal for the shotnoise-driven ratchet and for the ratchet with a continuous,

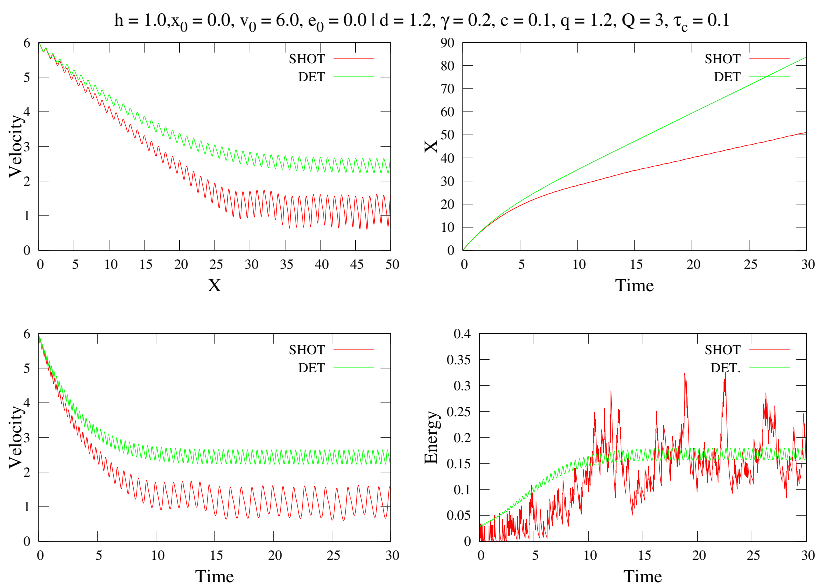

Fig. 9. Dynamics of particles on a flat Mateos' ratchet ($h = 1$), which is driven by Poissonian noise with mean distance between shots $\langle \delta t = 0.1 \rangle$. The left panels show the velocity energy as a function of the coordinated and of the time, respectively. The right panels show: above — the coordinate as a function of time and below — the energy content of the reservoir as a function of time. Each of the figures shows a comparison of the shotnoise-driven ratchet with a ratchet driven by a continuous input $q = 1.2$.

deterministic energy input. We note that the average velocity attained by particles moving in the system is lower for the shot-noise driven dynamics with respect to the case of a continuous and constant energy influx. In overall, we see that the efficiency of shot-noise driving in inducing transport properties of the system is much lower than for a deterministic case. We may muse that this situation improves in the region of possible synchrony.

A more careful theoretical investigation of the implications of shot noise in our model will be given in a separate work [31].

6. Conclusions and applications

We developed here the general schema of Hamiltonian systems coupled to energy reservoirs. As an application we studied the uphill motion of particles on ratchet-type potentials. We investigated the case when the support of external energy to the system is constant in intensity and continuous in time and compared this scenario with a situation when the support of energy is discrete and occurring randomly in time. The latter case was proposed to be modeled as an energetic shot noise. Possibly both models could be used to describe the energy support of biological systems and the conversion to mechanical or electrical work. Possible examples are the energy-converting systems as *e.g.* the ATPase [17, 18, 32].

Our model starts from the observation that there is in biology an elementary energetic act and ATP is the "energetic valuta of the cell". This means the source of all energetic processes in the cell are the absorption of energetic quanta carried by the molecule ATP (adenosine triphosphate acid). The molecule ATP contains 2 phosphate bindings which release in hydrolysis a large amount of free energy:

$$\mathrm{ATP} + \mathrm{H}_2 \rightarrow \mathrm{ADP} + P_i\,, \qquad \Delta G_0 = -31.8\,\mathrm{kJM}^{-1} \approx -13 k_{\mathrm{B}} T\,. \tag{50}$$

In the processes connected with the transformation of ATP–ADP in most cases a specific enzyme, the ATPase, is involved. This enzyme is the basic generator of work in form of proton-gradients. The ATPase is also an important enzyme working like a motor, which participates in proton and electron transport. It is connected with rotations and works in a 6-steps-regime. The rotations are stochastic and counterclockwise per 120° step. Under certain conditions the system may work also in opposite direction and generate ATP at the cost of mechanical or electrical work. This way ATP-synthase is also the basic generator of ATP molecules in the living organism. It synthesizes ATP from ADP and phosphate and is connected with a rotation clockwise. Both processes are related to each other as motor and dynamo in electrotechnics.

We do not claim that our model provides a realistic theory of the energy conversion processes discussed above. However, we assume that it could be used as possible schema supplementing existing models [18].

Standard models of molecular motors are based on the Smoluchowski equations for discrete systems having several states which correspond to attachment or detachment [17,18]. Many models have been developed which follow similar lines. We followed in this work another route which is based on Hamiltonian ratchets. We studied several Hamiltonian ratchets which are connected to an energy reservoir and gave special attention to possible applications to pumping processes as *e.g.* proton transfer. We investigated the motion of a particle against a gradient of the potential *i.e.* uphill motion under conditions where the external force is pointing downhill. The general schema is the following: chemical energy is absorbed and introduced into our "machine" increasing the reservoir of $e(t)$ by a certain amount. This is first modeled by a continuous inflow q and later in a more refined model or by discrete energy quanta, representing the absorption of one molecule ATP. Then the energy flows to the "motor" and is transformed into mechanical or electrical energy. This should model the increase of the energy of protons by transport through the membrane. We have shown that the particles on Hamiltonian ratchets driven by an uptake of energy from an energy reservoir are able to move uphill (in our case left to right), doing work and consuming reservoir energy $e(t)$ in an efficient way. The question remains how realistic our model is with respect to the proposed applications. We will address this issue in the forthcoming studies.

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REFERENCES

[1] Y.L. Klimontovich, *Statistical Theory of Open Systems*, Kluwer Academic Publ., Amsterdam 1997.

[2] W. Ebeling, I. Sokolov, *Statistical Thermodynamics and Stochastic Theory of Nonequilibrium Systems*, World Scientific, Singapore 2005.

[3] F. Schweitzer, W. Ebeling, B. Tilch, *Phys. Rev. Lett.* **80**, 5044 (1998).

[4] W. Ebeling, F. Schweitzer, B. Tilch, *BioSystems* **49**, 17 (1999).

[5] U. Erdmann, W. Ebeling, L. Schimansky-Geier, F. Schweitzer, *Eur. Phys. J.* **15**, 105 (2000).

[6] T. Vicsek, *Fluctuations and Scaling in Biology*, University Press, Oxford 2001.

[7] A.S. Mikhailov, V. Calenbuhr, *From Cells to Societies*, Springer Series in Synergetics, Springer, Berlin 2002.

[8] F. Schweitzer, *Brownian Agents and Active Particles*, Springer Series in Synergetics, Springer, Berlin 2003.

[9] A. Ordemann, F. Moss, G. Balaszi, *Motions of Daphnia in a Light Field: Random Walks with a Zooplankton* in F. Beck, M.T. Hütt, U. Lüttge (Eds.), Springer, 2003.

[10] W. Ebeling, *Acta Phys. Pol. B* **38**, 1657 (2007).

[11] W. Ebeling, L. Schimansky-Geier, *Eur. Phys. J. ST* **157**, 17 (2008).

[12] H. Haken, *Z. Phys.* **263**, 267 (1973).

[13] R. Graham, *Stochastic Models*, in Springer Tracts in Modern Physics, **66**, (1973); *Models of Stochastic Behaviour*, in S.B. Chen, B. Chu, R. Nossal (Eds.) *Scattering Technique*, Plenum Press, New York 1978.

[14] W. Ebeling, *Condens. Matter Phys.*, **3**, 285 (2000).

[15] F. Schweitzer, W. Ebeling, B. Tilch, *Phys. Rev.* **E64**, 02110-1-12 (2001).

[16] M. Smoluchowski, *Phys. Z.* **17**, 557 (1916).

[17] F. Jülicher, J. Prost, *Phys. Rev. Lett.* **75**, 2618 (1995); **78**, 4510 (1997).

[18] F. Jülicher, A. Ajdari, J. Prost, *Rev. Mod. Phys.* **69**, 1269 (1997).

[19] U. Erdmann, W. Ebeling, V.S. Anishchenko, *Phys. Rev.* **E65**, 061106 (2002).

[20] U. Erdmann, W. Ebeling, A. Mikhailov, *Phys. Rev.* **E71**, 051904 (2005).

[21] W. Ebeling, G. Röpke, *Physica D* **187**, 268 (2004).

[22] B. Tilch, F. Schweitzer, W. Ebeling, *Physica A* **273**, 293 (1999).

[23] F. Schweitzer, B. Tilch, W. Ebeling, *Eur. Phys. J.* **B14**, 157 (2000).

[24] J.L. Mateos, *Phys. Rev. Lett.* **84**, 258 (2000); *Acta Phys. Pol. B* **32**, 307 (2001).

[25] L. Machura, J. Łuczka, P. Talkner, P. Hänggi, *Acta Phys. Pol. B* **38**, 1855 (2007).

[26] A. Fiasconaro, W. Ebeling, E. Gudowska-Nowak, *Eur. Phys. J.* **B**, submitted.

[27] T. Czernik, J. Łuczka, *Ann. Phys. (Leipzig)* **9**, 721 (2005).

[28] I. Eliazar, J. Klafter, *Proc. Natl. Acad. Sci. (USA)* **27**, 13779 (2005).

[29] C. Kim, E.K. Lee, P. Hänggi, P. Talkner, *Phys. Rev.* **E76**, 011109 (2007).

[30] R. Zygadlo, *Phys. Rev.* **E47**, 4067 (1993).

[31] A. Fiasconaro, E. Gudowska-Nowak, W. Ebeling, in preparation.

[32] M. Bier, *Phys. Rev. Lett.* **91**, 148104 (2003).