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Active Brownian Particles with Internal Energy Depot

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Abstract

Active motion relies on the supply of energy. In order to turn passive into active motion, we need to consider mechanisms of energy take-up, storage and conversion. A suitable approach which considers both the energetic and stochastic aspects of active motion is provided by the model of Active Brownian particles. For a supercritical supply of energy these particles are able to move in a "high velocity" or active mode, which results in deviation from the Maxwellian velocity distribution. We investigate different types of complex motion of active Brownian particles moving in external potentials. Among the examples are the occurence of stochastic limit cycles, transitions between Brownian and directed motion, the "uphill" motion against the direction of an external force, or the establishment of positive or negative net currents in a ratchet potential, dependent on energy supply and stochastic influences.

1 Passive vs. Active Motion

The motion of a "simple" Brownian particle is due to fluctuations of the surrounding medium, i.e. the result of random impacts of the molecules or atoms of the liquid or gas, the particle is immersed in. This type of *undirected* motion would be rather considered as *passive* motion, simply because the Brownian particle does not play an active part in this motion. Passive motion can be also directed, if it is driven e.g. by convection, currents or by external fields.

Active motion, on the other hand relies on the supply of energy. Already in physico-chemical systems a *self-driven motion* of particles can be observed [1]. On the biological level, *active* self-driven motion can be found on different scales, ranging from cells [2] or simple microorganisms up to higher organisms, such as bird or fish. Last, but not least, also human movement can be described as active motion [3], as well as the motion of cars. All these types of active motion occur under energy consumption and energy conversion and may also involve processes of energy storage.

Recent investigations on *interacting* self-driven entities [4–6] focus on collective effects, such as the formation of swarms or crowds, rather than on the origin of the entities' velocity; i.e. it is usually postulated that the entities move with a certain non-zero velocity. In order to describe both the *random* aspects and the *energetic* aspects of active motion, we have introduced a model of *active Brownian particles* [7–11]. These are Brownian particles with the ability to take up energy from the environment, to store it in an internal depot and to convert internal energy to perform different activities, such as metabolism or motion. Possible changes of the environment or signal-response behavior are neglected here.

In order to turn passive (Brownian) motion into active motion, we need to consider mechanisms of energy take-up. A very simple mechanism is the pumping of energy by *space-dependent friction* [7] which in a certain spatial range can be also negative. Inside this area the Brownian particle, instead of loosing energy because of dissipative processes, is pumped with energy, which in turn increases its velocity. While such an approach will be able to model the spatially inhomogeneous supply of energy, it has the drawback not to consider processes of storage and conversion of energy. In fact, with only a space-dependent friction, the Brownian particle is instantaneously accelerated or slowed down, whereas e.g. biological entities or cars have the capability to stretch their supply of energy over a certain time interval.

In order to develop a more realistic model of active motion, we have considered an *internal energy depot* for the Brownian particles [10, 11], which allows to store the taken-up energy in the internal depot, from where it can be converted e.g. into kinetic energy, namely for the acceleration of motion. Additionally, the internal dissipation of energy, due to storage and conversion (or metabolism in a biological context) can be considered.

With these extensions, the Brownian particle becomes in fact a *Brownian motor* [12–14], which is fueled somewhere and then uses the stored energy with a certain efficiency [11] to move forward, also against external forces. Provided a supercritical supply of energy, we find that the motion of active Brownian particles in the two-dimensional space can become rather complex as shown in the sections below.

2 Pumping from an Internal Energy Depot

The motion of simple Brownian particles in a space-dependent potential, $U(\boldsymbol{r})$ can be described by the Langevin equation:

$$\dot{\boldsymbol{r}} = \boldsymbol{v}\,;\;\; m\,\dot{\boldsymbol{v}} = -\gamma_0 \boldsymbol{v} - \nabla U(\boldsymbol{r}) + \mathcal{F}(t) \tag{1}$$

where γ_0 is the friction coefficient of the particle at position $\boldsymbol{r}$, moving with velocity $\boldsymbol{v}$. $\mathcal{F}(t)$ is a stochastic force with strength D and a δ-correlated time dependence

$$\langle \mathcal{F}(t) \rangle = 0\,;\;\; \big\langle \mathcal{F}(t)\mathcal{F}(t') \big\rangle = 2D\,\delta(t-t') \tag{2}$$

Using the fluctuation-dissipation theorem, we assume that the loss of energy resulting from friction, and the gain of energy resulting from the stochastic force, are compensated in the average, and D can be expressed as $D = k_B T \gamma_0$, where T is the temperature and k_B is the Boltzmann constant.

In addition to the dynamics described above, the Brownian particles considered here are active in the sense that they are able to take up energy from the environment, which can be stored in an *internal depot*, e. $q(\boldsymbol{r})$ shall be the space-dependent flux of energy into the depot. The internal energy can be converted into kinetic energy with a rate $d(\boldsymbol{v})$ which should be a function of the actual velocity of the particle. Further, we consider internal dissipation, which is assumed to be proportional to the depot energy, c being the rate of energy loss. The resulting balance equation for the internal energy depot, e, of an active Brownian particle is then given by:

$$\frac{d}{dt}e(t) = q(\boldsymbol{r}) - c\, e(t) - d(\boldsymbol{v})\, e(t) \tag{3}$$

A simple ansatz for $d(\boldsymbol{v})$ reads $d(\boldsymbol{v}) = d_2 v^2$, with $d_2 > 0$. The energy conversion results in an additional acceleration of the Brownian particle in the direction of movement. Hence, the equation of motion has to consider an additional driving force, $d_2 e(t)\boldsymbol{v}$. In [10, 11], we have postulated a stochastic equation for pumped Brownian particles, which is consistent with the Langevin eq. (1):

$$\dot{\boldsymbol{r}} = \boldsymbol{v}\,;\ m\dot{\boldsymbol{v}} + \gamma_0 \boldsymbol{v} + \nabla U(\boldsymbol{r}) = d_2 e(t)\boldsymbol{v} + \mathcal{F}(t) \tag{4}$$

From now on, $m = 1$ is used. The Langevin eq. (4) can be rewritten in the known form, eq. (1), by introducing a *velocity-dependent friction coefficient*:

$$\gamma(\boldsymbol{v}) \quad = \quad \gamma_0 - d_2\, e(t) \tag{5}$$

Here, the value of $\gamma(\boldsymbol{v})$ changes dependent on the value of the internal energy depot, which itself is a function of the velocity. If the term $d_2\, e(t)$ exceeds the "normal" friction, γ_0, the velocity dependent friction coefficient can be negative which means the active particle's motion is pumped with energy. In order to get an estimate of the range of energy pumping, we assume a constant influx of energy into the internal depot, $q(\boldsymbol{r}) = q_0$, and a fast relaxation of the internal energy depot, eq. (3), which reads in an adiabatic approximation:

$$e_0 = \frac{q_0}{c + d_2 \boldsymbol{v}^2} \tag{6}$$

The quasistationary value e_0 can be used to appoximate the velocity-dependent friction coefficient, $\gamma(\boldsymbol{v})$, eq. (5):

$$\gamma(\boldsymbol{v}) = \gamma_0 - \frac{q_0\, d_2}{c + d_2 \boldsymbol{v}^2} \tag{7}$$

which is plotted in Fig. 1.

Dependent on the parameters γ_0, d_2, q_0, c the friction function, eq. (7), may have a zero, where the friction is just compensated by the energy supply. It reads in the considered case:

$$\boldsymbol{v}_0^2 = \frac{q_0}{\gamma_0} - \frac{c}{d_2} \tag{8}$$

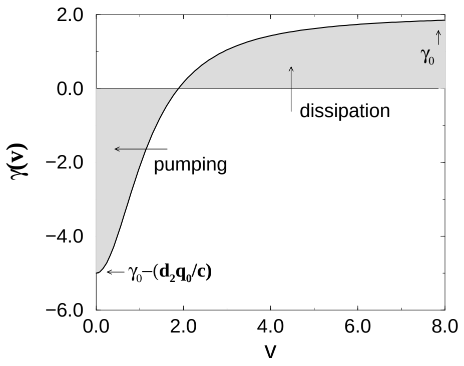

Figure 1: Velocity-dependent friction coefficient, $\gamma(\boldsymbol{v})$, eq. (7) vs. velocity $\boldsymbol{v}$. The velocity ranges for "pumping" ($\gamma(\boldsymbol{v}) < 0$) and "dissipation" ($\gamma(\boldsymbol{v}) > 0$) are indicated. Parameters: $q_0 = 10$; $c = 1.0$; $\gamma_0 = 20$, $d_2 = 10$. [16]

We see that for $\boldsymbol{v} < \boldsymbol{v}_0$, i.e. in the range of small velocities pumping due to negative friction occurs, as an additional source of energy for the Brownian particle. Hence, slow particles are accelerated, while the motion of fast particles is damped.

Due to the pumping mechanism discussed here, the conservation of energy clearly does not hold for the particle, i.e. we now have a non-equilibrium, canonical-dissipative system instead of an equilibrium canonical system. This should result in deviations from the known Maxwellian velocity distribution.

We restrict the further discussion to the two-dimensional space $\boldsymbol{r} = \{x_1, x_2\}$. Then the stationary velocities v_0, eq. (8), where the friction is just compensated by the energy supply, define a cylinder, $v_1^2 + v_2^2 = \boldsymbol{v}_0^2$, in the four-dimensional state space $\{x_1, x_2, v_1, v_2\}$ which attracts all deterministic trajectories of the dynamic system [16]. The probability density for the velocity, $P(\boldsymbol{v}, t)$, can be described by a Fokker-Planck equation, which reads for the friction function, eq. (7), and in the absence of an external potential, i.e. $U(x_1, x_2) \equiv 0$:

$$\frac{\partial P(\boldsymbol{v},t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{v}} \left[\left(\gamma_0 - \frac{d_2 q_0}{c + d_2\, \boldsymbol{v}^2} \right) \boldsymbol{v}\, P(\boldsymbol{v},t) + D\, \frac{\partial P(\boldsymbol{v})}{\partial v} \right] \tag{9}$$

The stationary solution of eq. (9) yields:

$$P^0(\boldsymbol{v}) = C \left(1 + \frac{d_2 \boldsymbol{v}^2}{c} \right)^{\frac{q_0}{2D}} \exp\left(-\frac{\gamma_0}{2D}\, \boldsymbol{v}^2 \right) \tag{10}$$

where C results from the normalization condition. Compared to the Maxwellian velocity distribution of "simple" Brownian particles, a new prefactor appears now in eq. (10) which results from the internal energy depot. In the range of small values of $\boldsymbol{v}^2$, the prefactor can be expressed by a power

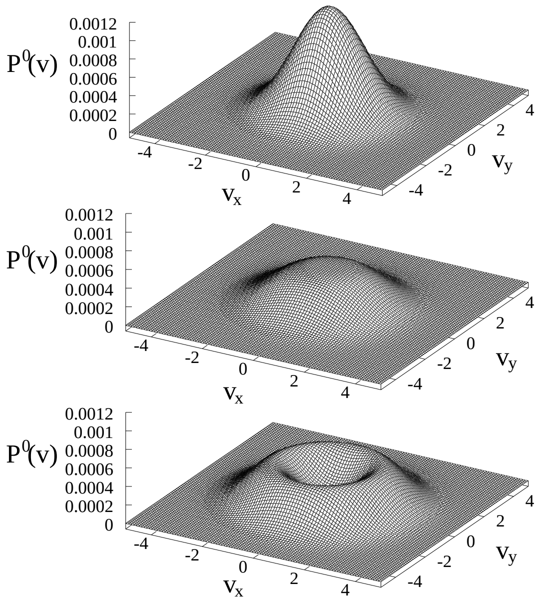

Figure 2: Normalized stationary solution $P^0(\boldsymbol{v})$, eq. (10), for $d_2 = 0.07$ (top), $d_2 = 0.2$ (middle) and $d_2 = 0.7$ (bottom). Other parameters: $\gamma_0 = 2$, $D = 2$, $c = 1$, $q_0 = 10$. Note that $d_2 = 0.2$ is the bifurcation point for the given set of parameters. [16]

series truncated after the first order, and eq. (10) reads then:

$$P^0(\boldsymbol{v}) \sim \exp\left[-\frac{\gamma_0}{2D}\left(1 - \frac{q_0 d_2}{c\gamma_0}\right)\boldsymbol{v}^2 + \cdots\right] \tag{11}$$

In eq. (11), the sign of the expression in the exponent depends significantly on the parameters which describe the balance of the energy depot. For a subcritical pumping of energy, $q_0 d_2 < c\gamma_0$, the expression in the exponent is negative and an *unimodal velocity distribution* results, centered around the maximum $\boldsymbol{v}_0 = 0$. This corresponds to the *Maxwellian velocity distribution*. However, for supercritical pumping,

$$q_0 d_2 > c\gamma_0 \tag{12}$$

the exponent in eq. (11) becomes positive, and a *crater-like velocity distribution* results, which indicates strong deviations from the Maxwell distribution (cf. Fig. 2). The maxima of $P^0(\boldsymbol{v})$ correspond to the solutions for $\boldsymbol{v}_0^2$, eq. (8).

3 Motion in a Parabolic Potential

In the following we discuss the motion of a Brownian particle with an internal energy depot in a two-dimensional parabolic potential:

$$U(x_1, x_2) = \frac{a}{2}(x_1^2 + x_2^2) \tag{13}$$

This potential originates a force directed to the minimum of the potential, however, the random force in eq. (4) keeps the particle moving, even without the take-up of energy (cf. Fig. 3). If we consider a take-up of energy which is constant in space, $q(x_1, x_2) = q_0$, Fig. 3 demonstrates that the particle reaches out farther, moving on a stochastic limit cycle, if some critical conditions are satisfied. In [11] it was shown that for the case of the harmonic potential these critical conditions coincide with those obtained for $U(x_1, x_2) \equiv 0$, i.e. eq. (12) has to be fulfilled again.

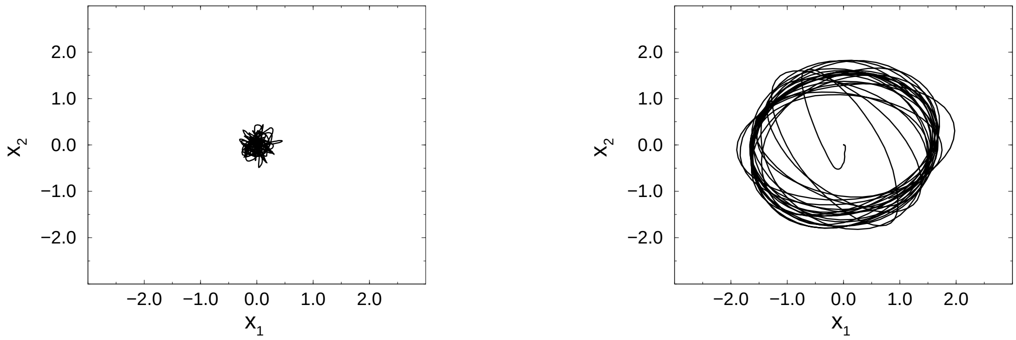

Figure 3: Stochastic motion of an active Brownian particle in a parabolic potential. (left) $q = 0$ (simple Brownian motion), (right) $q_0 = 1.0$ (other parameters: $\gamma_0 = 0.2$ $d_2 = 1.0$, $c = 0.1$, $D = 0.01$, $a = 2$, initial conditions: $(x_1, x_2) = (0, 0)$, $(v_1, v_2) = (0, 0)$, $e(0) = 0$). [10]

If we consider that the energy influx is not constant, but space dependent, for example

$$q(x_1, x_2) = \begin{cases} q_0 & \text{if } \left[(x_1 - b_1)^2 + (x_2 - b_2)^2\right] \leq R^2 \\ 0 & \text{else} \end{cases} \tag{14}$$

then the internal depot of the active Brownian particles can be refilled only in a restricted area. Eq. (14) assumes that the supply area (*energy source*) is modeled as a circle, the center being different from the minimum of the potential. Noteworthy, the active particle is *not* attracted by the energy source due to long-range attraction forces. In the beginning, the internal energy depot of the particle is empty and active motion is not possible. So, the particle may hit the supply area because of the action of the stochastic force. But once the energy depot is filled up, it increases the particles motility, as presented in Fig. 4. Most likely, the motion into the energy area becomes accelerated,

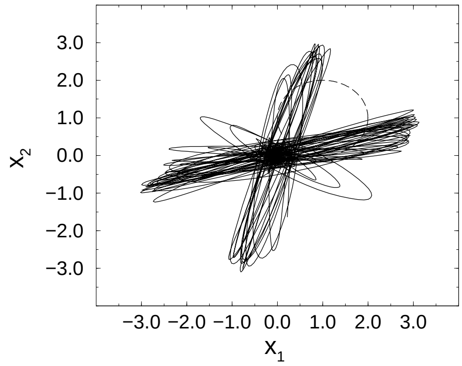

Figure 4: Trajectories in the x_1, x_2 space for the stochastic motion of an active Brownian particle in a parabolic potential. The circle (cooordinates (1,1), radius $R = 1$) indicates the area of energy supply, eq. (14). Parameters: $d_2 = 1$, $q_0 = 10$, $\gamma_0 = 0.2$, $c = 0.01$, $D = 0.01$, $a = 2$, initial conditions: $(x_1, x_2) = (0, 0)$, $(v_1, v_2) = (0, 0)$, $e(0) = 0$. [10]

therefore an oscillating movement between the energy source and the potential minimum occurs after an initial period of stabilization.

Interestingly, the oscillating motion breaks down after a certain time. Then the active particle, with an empty internal depot, moves again like a simple Brownian particle, until a new cycle starts, as indicated in Fig. 4. This way the particle motion is of intermittent type. We found that the trajectories eventually cover the whole area inside certain boundaries, however during an oscillation period the direction is most likely kept.

We may also consider that active motion occurs in more complex landscapes which typically not only contain localized areas of energy supply, but also *obstacles*. We have discussed such a case while assuming a hard-core like obstacle where the particle is simply reflected at the boundary if it hits the obstacle. Considering a continuous supply of energy but only a deterministic motion, we found a chaotic motion of the active particle in the phase space $\Gamma = \{x_1, x_2, v_1, v_2, e\}$ [10]. Hence, we concluded that for the motion of Brownian particles with energy depots reflecting obstacles have an effect similar to stochastic influences (external noise).

4 Motion in a Linear/Periodic Potential

In the following, we restrict the discussion to the *one-dimensional case*, i.e. the space coordinate is given by x. For the potential, we assume a linear function, $U(x) = ax$, hence the resulting force is a constant: $\boldsymbol{F} = -\boldsymbol{\nabla} U = -a$. Further the flux of energy into the internal depot of the particle is assumed as constant, $q(x) = q_0$. Then, the dynamics for the pumped Brownian motion is described by the following set of equations:

$$\begin{aligned} \dot{\boldsymbol{v}} &= -\big(\gamma_0 - d_2 e(t)\big)\boldsymbol{v} + \boldsymbol{F} + \sqrt{2D}\boldsymbol{\xi}(t) \\ \dot{e} &= q_0 - ce - d_2 \boldsymbol{v}^2 e \end{aligned} \tag{15}$$

In the deterministic case, the stationary solutions of eq. (15) obtained from $\dot{\boldsymbol{v}} = 0$ and $\dot{e} = 0$ lead to a cubic polynom for the velocity $\boldsymbol{v}_0$:

$$d_2\gamma_0\boldsymbol{v}_0^3 - d_2\boldsymbol{F}v_0^2 - (q_0 d_2 - c\gamma_0)\boldsymbol{v}_0 - c\boldsymbol{F} = 0. \tag{16}$$

Here $\boldsymbol{v}_0^{n+1}$ is defined as a vector $|v_0|^n\,\boldsymbol{v}_0$. Depending on the value of F and in particular on the sign of the term $(q_0 d_2 - c\gamma_0)$, eq. (16) has either one or three real solutions for the stationary velocity, $\boldsymbol{v}_0$. This is also shown in the bifurcation diagram, Fig. 5.

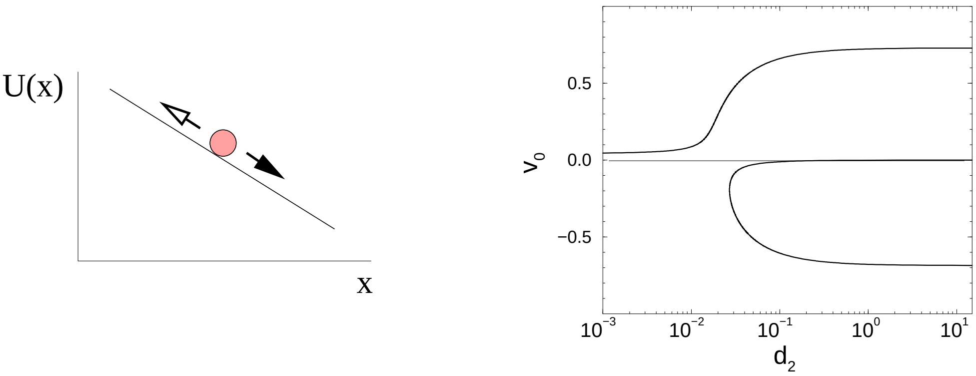

Figure 5: (right) Sketch of the one-dimensional motion of the particle in the presence of a constant force $\boldsymbol{F} = -\boldsymbol{\nabla}U(x)$ =const. Provided a supercritical amount of energy from the depot, the particle might be able to move “uphill”, i.e. against the direction of the force. (left) Stationary velocities $\boldsymbol{v}_0$, eq. (16), vs. conversion rate d_2. Above a critical value of d_2, a negative stationary velocity indicates the posssibility to move against the direction of the force. Parameters: $\boldsymbol{F} = +7/8$, $q_0 = 10$, $\gamma_0 = 20$, $c = 0.01$. [17]

The always existing solution expresses a direct response to the force in the form: $\boldsymbol{v}_0 \sim \boldsymbol{F}$, i.e. it results from the analytic continuation of Stokes’ law, $\boldsymbol{v}_0 = \boldsymbol{F}/\gamma_0$, which is valid for $d_2 = 0$. We denote this solution as the “normal” mode of motion, since the velocity $\boldsymbol{v}$ has the same direction as the force $\boldsymbol{F}$ resulting from the external potential $U(x)$.

As long as the supply from the energy depot is small, we will also name the normal mode as the *passive mode*, because the particle is simply driven by the external force. More interesting is the case of three stationary velocities, $\boldsymbol{v}_0$, which significantly depends on the (supercritical) influence of the energy depot. In this case the particle will be able to move in a “high velocity” or *active mode* of motion. Fig. 5 shows that the former passive normal mode, which holds for subcritical energetic conditions, is transformed into an active normal mode, where the particle moves into the same direction, but with a much higher velocity. *Additionally*, in the active mode a new high-velocity motion *against* the direction of the force $\boldsymbol{F}$ becomes possible, which corresponds to an "uphill" motion.

It is obvious that the particle's motion "downhill" is stable, but the same does not necessarily apply for the possible solution of an "uphill" motion. In [17], we have investigated the necessary conditions for such a motion in a linear potential. For the *deterministic* case, we found the following critical condition for a possible "uphill" motion of the pumped Brownian particle:

$$d_2^{crit} = \frac{F^4}{8q_0^3}\left(1+\sqrt{1+\frac{4\gamma_0 q_0}{F^2}}\right)^3 \tag{17}$$

In the limit of negligible internal dissipation $c \to 0$, eq. (17) describes how much power has to be supplied by the internal energy depot to allow a *stable uphill motion* of the particle.

This result will be used to explain the motion of an *ensemble* of N active Brownian particles in a piecewise linear, asymmetric potential (cf. Fig. 6), which is known as a *ratchet potential* [14, 15].

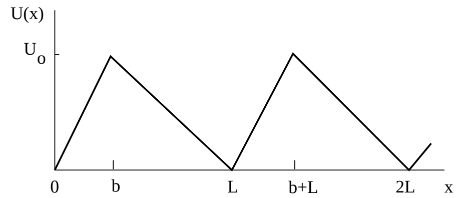

Figure 6: Sketch of the ratchet potential $U(x)$. For the computer simulations, the following values are used: b=4, L=12, $U_0 = 7$ in arbitrary units.

Fig. 7 shows the *net current* expressed by the mean velocity $\langle v \rangle$, dependent on the conversion rate, d_2. For the *determinstic motion* ($D = 0$), we see the existence of *two different critical values* for the parameter d_2. For values of d_2 near zero and less than d_2^{crit1}, there is no net current at all. This is due to the subcritical supply of energy from the internal depot, which does not allow an uphill motion on any flank of the potential. With an increasing value of d_2, we see the occurence of a negative net current at d_2^{crit1}. That means, the energy depot provides enough energy for the uphill motion along the flank with the lower slope. For $d_2^{crit1} \leq d_2 \leq d_2^{crit2}$, a stable motion of the particles up and down the flank with the lower slope is possible, but not for the steeper slope. Only for $d_2 > d_2^{crit2}$, the energy depot also supplies enough energy for the particles to climb up the steeper slope, consequently a periodic motion of the particles into the positive direction becomes possible, now.

For the computer simulations, we have assumed that the start locations of the particles are equally distributed over the first period of the potential, $\{0, L\}$ and their initial velocity is zero. Hence,

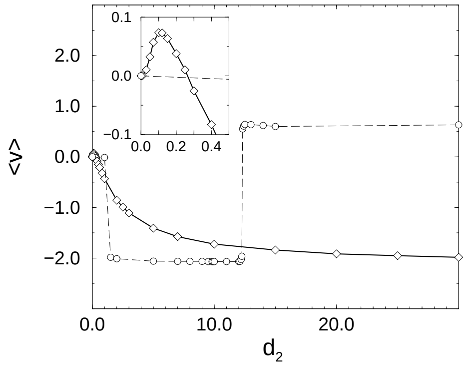

Figure 7: Average velocity $\langle v \rangle$ vs. conversion parameter d_2. The data points are obtained from simulations of 10.000 particles with arbitrary initial positions in the first period of the ratchet potential. ($\diamond$) stochastic case ($D = 0.1$), ($\circ$) deterministic case ($D = 0$). Parameters: $q_0 = 1.0$, $\gamma_0 = 0.2$, $c = 0.1$. [18]

with respect to Fig. 6 more particle start into the positive direction, which eventually results in a larger positive net current for $d_2 > d_2^{crit2}$ [18]. If we insert the two different values for F (cf. Fig. 6) into the critical condition, eq. (17), we find for the critical values $d_2^{crit1} = 1.03$ and $d_2^{crit1} = 11.3$, which agrees with the onset of the negative and the positive current in the deterministic computer simulations, Fig. 7.

In the deterministic case, the particles will keep their direction determined by the initial conditions provided the energy supply allows them to move "uphill". In the stochastic case, however, the initial conditions will be "forgotten" after a short time, hence due to stochastic influences the particle's "upill" motion along the steeper flank will soon turn into a "downhill" motion. In [18], we have investigated the two-dimensional separatrix plane, which separates the motion into positive and negative directions in the threedimensional phase space, $\{x, v, e\}$. We found that, if a particle moves into the positive direction, most of the time the trajectory is very close to the separatrix. That means it will be rather susceptible for small perturbations, i.e. even small fluctuations might be able to destabilize the motion into the positive direction. The motion into negative direction, on the other hand, is not susceptible in the same manner, since the respective trajectory remains in a considerable distance from the separatrix or comes close to the separatrix only for a very short time.

Thus, the stochastic fluctuations reveal the instability of the motion into the positive direction, i.e. the "uphill" motion along the *steeper* slope. Hence, in the stochastic case the net current is always negative. In addition, we find a *very small* positive net current in the range of small d_2 (cf. the insert in Fig. 7), because the fluctuations allow some particles to escape the potential barriers.

In order to investigate how much the strength D of the stochastic force may influence the magnitude of the net current into the negative direction, we have varied D for a fixed conversion parameter

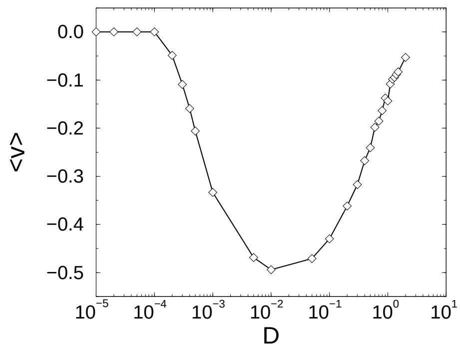

Figure 8: Average velocity $\langle v \rangle$ vs. strength of the stochastic force D. The data points are obtained from simulations of 10.000 particles with a fixed conversion parameter $d_2 = 1.0$, for the other parameters see Fig. 7. [18]

$d_2 = 1.0$. As Fig. 7 indicates, for this setup there will be only a negligible net current, $\langle v \rangle \approx 0$ in the deterministic case ($D = 0$), but a remarkable net current, $\langle v \rangle = -0.43$ in the stochastic case for $D = 0.1$. As Fig. 8 shows, there is a *critical strength* of the stochastic force, $D^{crit}(d_2 = 1.0) \simeq 10^{-4}$, where an onset of the net current can be observed, while for $D < D^{crit}$ no net current occurs. On the other hand, there is also an *optimal strength* of the stochastic force, D^{opt}, where the amount of the net current, $|\langle v \rangle|$, reaches a *maximum*. An increase of the stochastic force above D^{opt} will only increase the *randomness* of the particle's motion, hence the net current decreases again. In conclusion, this sensitive dependence on the stochastic force may be used to adjust a *maximum net current* for the particles movement in the ratchet potential.

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