Directed motion of Brownian particles with internal energy depot

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Abstract

A model of Brownian particles with the ability to take up energy from the environment, to store it in an internal depot, and to convert internal energy into kinetic energy of motion, is discussed. The general dynamics outlined in Sect. 2 is investigated for the deterministic and stochastic particle's motion in a non-fluctuating ratchet potential. First, we discuss the attractor structure of the ratchet system by means of computer simulations. Dependent on the energy supply, we find either periodic bound attractors corresponding to localized oscillations, or one/two unbound attractors corresponding to directed movement in the ratchet potential. Considering an ensemble of particles, we show that in the deterministic case two currents into different directions can occur, which however depend on a supercritical supply of energy. Considering stochastic influences, we find the current only in one direction. We further investigate how the current reversal depends on the strength of the stochastic force and the asymmetry of the potential. We find both a critical value of the noise intensity for the onset of the current and an optimal value where the net current reaches a maximum. Eventually, the dynamics of our model is compared with other ratchet models previously suggested.

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1 Introduction

Among the phenomena presently investigated in cell biology is the generation of directed movement of “particles” (e.g. kinesin or myosin molecules) along periodic structures (e.g. microtubules or actin...
filaments) [1] in the absence of a macroscopic force, which may have resulted from temperature or concentration gradients. In order to reveal the microscopic mechanisms resulting in directed movement, different physical ratchet models have been proposed [2], such as forced thermal ratchets [3], or stochastic ratchets [4, 5], or fluctuating ratchets [6, 7]. These models are based on different types of long-range order correlations, e.g. a periodic asymmetric potential, or a time-dependent change of noise, or a fluctuating energy barrier (cf. also Sect. 4). They have in common to transfer the undirected motion of Brownian particles into a directed motion, hence, the term Brownian rectifiers [8] has been established.

The ratchet models have recently proved their value for describing Brownian machines or molecular motors [9–11], which convert chemical energy into mechanical motion. The model discussed in this paper, aims to add a new perspective to this problem. Our model is based on active Brownian particles [12–17], which 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, motion, change of the environment, or signal-response behavior. In this paper, we focus on the energetic aspects of the motion of these active Brownian particles in a specific potential and neglect the possible changes of the environment.

Different from “usual” Brownian particles which only move passively caused by the influence of a stochastic force, active Brownian particles have the capability of active motion. This means for instance the possibility of accelerated motion, provided there is a supercritical supply of energy from the environment. In general, we can think of different mechanisms to pump additional energy into the motion of the particles. For example, a complex friction coefficient, \(\gamma(r, v)\), can be considered, which is a space- and /or velocity dependent function, which can be also negative under certain conditions. Space-dependent negative friction has been discussed in [13], while different ansatzes for a complex velocity-dependent friction coefficient are investigated in [17, 18]. It can be shown that above a critical influx of energy the Brownian particles are able to perform a selfsustained limit cycle motion.

In our model, the Brownian particles are not just pumped by additional energy, but also have the capability to store energy in an internal depot. This means an additional degree of freedom for the particle, which may allow a simplified description of active biological motion on the microlevel [17]. Considering for instance a spatially inhomogeneous supply of energy, or the presence of obstacles, we have shown that the motion of active Brownian particles in the two-dimensional space can become rather complex [16]. We have found e.g. intermittent types of motion where cycles of accelerated motion alternate with cycles of “simple” Brownian motion, or deterministic chaos in the presence of reflecting obstacles.

In this paper, we investigate the motion of an ensemble of Brownian particles with internal energy depot in a ratchet potential, i.e. a periodic potential which lacks the reflection symmetry. In Sect. 2, we discuss the basic features of our model and derive the equations of motion and the stationary solutions for the case of a linear potential. In Sect. 3, we specify the external potential as a
non-fluctuating ratchet potential. By means of computer simulations, we investigate the attractor structure of the particles motion and show the existence of bound and unbound attractors dependent on the energy supply. Further, we compare the deterministic motion of the particle ensemble with the stochastic motion. We show that in the deterministic case a positive net current occurs, which changes its direction in the presence of stochastic influences. In order to investigate the current reversal in more detail, in Sect. 4 the dependence of the net current on the energy supply and the asymmetry of the potential is calculated both for the deterministic and the stochastic case. In Sect. 5, we compare our model with different ratchet models suggested previously, and point to some differences.

2 Model of Pumped Brownian Dynamics

2.1 Equations of Motion and Distribution Function

The model of active Brownian motion investigated in this paper is based on the idea [16, 17] that the particles have the capability to store energy in an internal energy depot, $e(t)$, which may be changed due to three different processes:

(i) gain of energy from the environment, where $q(r)$ is the flux of energy into the depot. If the availability of energy is inhomogeneously distributed, the energy flux may depend on the space coordinate, $r$.

(ii) loss of energy due to internal dissipation, which is assumed to be proportional to the internal energy. Here the rate of energy loss, $c$, is assumed to be constant.

(iii) conversion of internal energy into kinetic energy with a rate $d(v)$, which should be a function of the actual velocity, $v$, of the particle.

The resulting balance equation for the energy depot is given by:

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

(1)

A simple ansatz for $d(v)$ reads:

$$d(v) = d_2 v^2 ; \quad d_2 > 0$$

(2)

If we consider the motion of a particle with mass $m$ in an external potential, $U(r)$, the balance equation for the mechanical energy $E_0$ of the particle reads:

$$\frac{d}{dt}E_0(t) = \frac{d}{dt} \left( \frac{1}{2} m v^2 + U(r) \right) = \left( \eta(v^2) d_2 e(t) - \gamma_0 \right) v^2$$

(3)

It means that $E_0$ can be changed by two processes:
1. increase of the kinetic energy by conversion of depot energy, where \( \eta(v^2) \leq 1 \) is the conversion efficiency

2. decrease by dissipation of energy due to the friction, \( \gamma_0 \), of the moving particle.

Based on Eq. (3), we postulate a stochastic equation of motion for pumped Brownian particles [16, 17] which is consistent with the known Langevin equation of Brownian motion:

\[
m \dot{v} + \gamma_0 v + \nabla U(r) = \eta(v^2)d_2e(t)v + \sqrt{2D} \xi(t)
\]  

(4)

The right-hand side of the Langevin equation contains two driving forces for the motion:

1. the acceleration in the direction of movement, \( e_v = v/v \), due to the conversion of internal into kinetic energy,

2. a stochastic force with the strength \( D \) and white-noise fluctuations: \( \langle \xi(t)\xi(t') \rangle = \delta(t-t') \).

According to the fluctuation-dissipation theorem, we assume that \( D \) can be expressed as:

\[
D = k_B T \gamma_0
\]

(5)

Because the loss of energy resulting from friction and the gain of energy resulting from the stochastic force are compensated in the average, the balance equation for the mechanical energy, Eq. (3), reads for the stochastic case:

\[
\left\langle \frac{d}{dt} \left( \frac{1}{2}mv^2 + U(r) \right) \right\rangle = \langle \eta(v^2)d_2e(t)v^2 \rangle
\]

(6)

The presence of an internal energy depot means an additional degree of freedom for the particle, which extends the phase space \( \Gamma = \{r, v, e\} \). Let \( p(r, v, e, t) \) denote the probability density to find the particle at time \( t \) at location \( r \) with velocity \( v \) and internal depot energy \( e \). The time-dependent change of the probability density can be described by a Fokker-Planck equation, which has to consider now both the Langevin Eq. (4) for the motion of the particle, and the equation for the energy depot, Eq. (1):

\[
\frac{\partial p(r, v, e, t)}{\partial t} = \frac{\partial}{\partial v} \left\{ \frac{\gamma_0 - \eta d_2e}{m} v p(r, v, e, t) + \frac{D}{m^2} \frac{\partial p(r, v, e, t)}{\partial v} \right\} - v \frac{\partial p(r, v, e, t)}{\partial r} + \frac{1}{m} \nabla U(r) \frac{\partial p(r, v, e, t)}{\partial v} - \frac{\partial}{\partial e} \left[ q(r) - c e - \eta d_2v^2e \right] p(r, v, e, t)
\]

(7)

For this probability density, the following normalization condition holds:

\[
\int_{-\infty}^{\infty} dr \int_{-\infty}^{\infty} dv \int_{0}^{\infty} de \ p(r, v, e, t) = 1
\]

(8)
In the following section, we will give the stationary solution for $p(r,v,e,t)$ for a particular potential. A more detailed discussion of the features of the probability density for pumped Brownian particles is given in [18].

### 2.2 Motion in a linear Potential

In the following, we restrict the discussion to the one-dimensional case, i.e. the space coordinate is given by $x$. Further the mass of the particle is set to $m = 1$ and the flux of energy into the internal depot of the particle is assumed as constant: $q(r) = q_0$. For the potential, we assume a linear function, hence the resulting force is a constant:

$$U(x) = ax; \quad F = -\nabla U = -a = \text{const.} \quad (9)$$

Then, the dynamics for the pumped Brownian motion is described by the following set of equations:

$$\begin{align*}
\dot{x} &= v \\
\dot{v} &= -\left(\gamma_0 - \eta(v^2)\right) v + F + \sqrt{2D}\xi(t) \\
\mu \dot{e} &= q_0 - ce - d_2 v^2 e
\end{align*} \quad (10)$$

Here, we have introduced a formal parameter $\mu$ which can be used to describe the time scale of relaxation of the internal energy depot. The limit $\mu \to 0$ describes a very fast adaptation of the depot. Assuming further an ideal efficiency, $\eta = 1$, we get as an adiabatic approximation for the energy depot:

$$e_0 = \frac{q_0}{c + d_2 v^2} \quad (11)$$

This allows us to rewrite the equations of motion as:

$$\begin{align*}
\dot{x} &= v \\
\dot{v} &= -\gamma(v^2) v + F + \sqrt{2D}\xi(t)
\end{align*} \quad (12)$$

where $\gamma(v^2)$ is a non-linear friction function:

$$\gamma(v^2) = \gamma_0 - \frac{d_2 q_0}{c + d_2 v^2} \quad (13)$$

In the limit of large velocities, $\gamma(v^2)$ approaches the normal friction coefficient, $\gamma_0$, whereas in the limit of small velocities a 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. A more detailed discussion of $\gamma(v^2)$ is given in [18].

A similar discussion holds if we assume that the value of the energy depot $e_0$ is constant and the conversion efficiency $\eta(v^2)$ decreases as follows with increasing velocity:

$$\eta(v^2) = \frac{\eta_1}{1 + \eta_2 v^2} \quad (14)$$
where $\eta_1$ and $\eta_2$ are constants. Then we find for the non-linear friction function with $\eta_0 = \eta_1 d_2$:

$$\gamma(v^2) = \gamma_0 - \frac{\eta_0 e_0}{1 + \eta_2 v^2}$$

which is a special case of Eq. (13). In the following, we will assume a constant conversion efficiency, $\eta(v^2) = 1$, and pay particular attention to the conversion parameter $d_2$, instead.

If we first discuss the overdamped limit, we can assume a fast relaxation of the velocities, in which case the set of equations, (10), can be further reduced to:

$$v(t) = \frac{1}{\gamma_0 - d_2 e_0} F + \sqrt{\frac{2 k_B T \gamma_0}{\gamma_0 - d_2 e_0}} \xi(t)$$

(16)

We note that, due to the dependence of $e_0$ on $v^2 = \dot{x}^2$, Eq. (16) is coupled to Eq. (11). Thus, the overdamped Eq. (16) could be also written in the form:

$$\left(\gamma_0 - d_2 \frac{q_0}{c + d_2 \dot{x}^2}\right) \dot{x} = F + \sqrt{2 k_B T \gamma_0} \xi(t)$$

(17)

Eq. (17) indicates a cubic equation for the velocities in the overdamped limit, i.e. the possible existence of non-trivial solutions for the stationary velocity. If we denote the stationary values of $v(t)$ by $v_0$ and neglect for the moment the stochastic term, Eq. (17) can then be rewritten as:

$$\left[d_2 \gamma_0 v_0^2 - (q_0 d_2 - c \gamma_0)\right] v_0 - d_2 F = c F.$$ (18)

Depending on the value of $F$ and in particular on the sign of the term $(q_0 d_2 - c \gamma_0)$, Eq. (18) has either one or three real solutions for the stationary velocity, $v_0$. The always existing solution expresses a direct response to the force in the form:

$$v_0 \sim F$$

(19)

This solution results from the analytic continuation of Stokes’ law, $v_0 = F/\gamma_0$, which is valid for $d_2 = 0$. We will denote this solution as the “normal” mode of motion, since the velocity $v$ has the same direction as the force $F$ resulting from the external potential $U(x)$.

As long as the supply of 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, $v_0$, which significantly depends on the (supercritical) influence of the energy depot. In this case which will be also discussed in the following sections, the particle will be able to move in a “high velocity” or active mode of motion.

For the one-dimensional motion, in the active mode only two different directions are possible, i.e. a motion into or against the direction of the force $F$. Considering the linear potential $U(x)$, Eq. (9), 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. Thus, in addition to Eq. (18) which provides the values of the stationary solutions, we need a second condition which guarantees the stability of these solutions. In [19], we have investigated the necessary conditions for such a motion in a linear potential. For the deterministic case, we found the following critical condition a possible “uphill” motion of the pumped Brownian particles:

\[ d_2^{\text{crit}} = \frac{F^4}{8q_0^3} \left( 1 + \sqrt{1 + \frac{4\gamma_0 q_0}{F^2}} \right)^3 \]  

(20)

d_2 is the conversion rate of internal into kinetic energy, and \( F = -\nabla U \) describes the constant slope of the potential. In the limit of negligible internal dissipation \( c \to 0 \), Eq. (20) describes how much power has to be supplied by the internal energy depot to allow a stable uphill motion of the particle.

In the following section, we will apply these results to a more sophisticated potential. But before, we want to give a formal solution for the Fokker-Planck Eq. (7) for the considered case \( F = \text{const.} \). If we neglect the space coordinate and concentrate on the distribution function \( p(v, e, t) \) instead, the stationary solution \( p^0(v, e) \) results from the following equation:

\[
\frac{\partial}{\partial v} \left\{ \left( \gamma_0 - d_2 e \right) v p(v, e) + D \frac{\partial p(v, e)}{\partial v} - F p(v, e) \right\} = \\
\frac{\partial}{\partial e} \left[ q_0 - c e - d_2 v^2 e \right] p(v, e)
\]

(21)

If we fix the depot energy \( e \) to the value \( e_0 \), Eq. (11), the stationary solution reads for sufficiently weak forces \( F \):

\[
p^0(v, e) \sim \delta(e - e_0) \left( c + d_2 v^2 \right)^{q_0/2} e^{\frac{-\gamma_0}{2D}} \exp \left[ -\frac{\gamma_0}{2D} \left( v - \frac{F}{\gamma_0} \right)^2 \right]
\]

(22)

where \( \delta(e - e_0) \) is Dirac’s delta function. An investigation of the possible stationary states in the full \( \{v, e\} \) phase space is given in [19].

3 Pumped Brownian Motion in a Ratchet Potential

3.1 Investigation of Deterministic Phase-Space Trajectories

For further investigations of the motion of pumped particles by means of computer simulations, we specify the potential \( U(x) \) as a piecewise linear, asymmetric potential (cf. Fig. 1), which is known
as a ratchet potential:

\[ U(x) = \begin{cases} 
\frac{U_0}{b} (x - nL) & \text{if } nL \leq x \leq nL + b \\
\frac{U_0}{L - b} ((n + 1)L - x) & \text{if } nL + b \leq x \leq (n + 1)L 
\end{cases} \]

(23)

Further, we will use the following abbreviations with respect to the potential \( U(x) \), Eq. (23). The index \( i = \{1, 2\} \) refers to the two pieces of the potential, \( l_1 = b \), \( l_2 = L - b \). The asymmetry parameter \( a \) should describe the ratio of the two pieces, and \( F = -\nabla U = \text{const.} \) is the force resulting from the gradient of the piecewise linear potential. Hence, for the potential \( U(x) \), Eq. (23), the following relations yield:

\[ F_1 = -\frac{U_0}{b} ; \quad F_2 = \frac{U_0}{L - b} ; \quad a = \frac{l_2}{l_1} = \frac{L - b}{b} = \frac{F_1}{F_2} \]

\[ F_1 = -\frac{U_0}{L} (1 + a) ; \quad F_2 = \frac{U_0}{L} \frac{1 + a}{a} \]

(24)

The motion of the Brownian particles with internal energy depot is still described by the set of equations, (10). In order to elucidate the class of possible solutions for the dynamics specified, let us first discuss the phase-space trajectories for the deterministic motion, i.e. \( D = 0 \). Further, \( \mu = 1 \) and \( \eta = 1 \) is assumed.

Due to friction, a particle moving in the ratchet potential, will eventually come to rest in one of the potential wells, because the dissipation is not compensated by the energy provided from the internal energy depot. The series of Fig. 2 shows the corresponding attractor structures for the particle’s motion dependent on the supply of energy expressed in terms of the conversion rate \( d_2 \).

In Fig. 2a, we see that for a subcritical supply of energy expressed in terms of the conversion rate \( d_2 \) only localized states for the particles exist. The formation of limit cycles inside each minimum corresponds to stable oscillations in the potential well, i.e. the particles are not able to escape from the potential well.

With increasing \( d_2 \), the particles are able to climb up the potential flank with the lower slope, and this way escape from the potential well into negative direction. As Fig. 2b shows, this holds also for particles which initially start into the positive direction. Thus, we find an unbound attractor corresponding to delocalized motion for negative values of \( v \). Only if the conversion rate \( d_2 \) is large enough to allow the uphill motion along the flank with the steeper slope, the particles can escape from the potential well in both directions, and we find two unbound attractors corresponding to delocalized motion into both positive and negative direction.

To conclude these investigations, we find that the structure of the phase space of a active Brownian particle in an unsymmetrical ratchet potential may be rather complex. While at low pumping rates bound attractors (limit cycles) in each potential well are observed, with increasing pumping rates
one/two new unbound attractors are formed, which correspond to a directed stationary transport of the particles into negative/positive direction.

Considering the three-dimensional phase space, \( \{x, v, e\} \), these two stationary solutions are separated by a two-dimensional separatrix plane. This plane has to be periodic in space because of the periodicity of the ratchet potential. In order to get an idea of the shape of the separatrix we have performed computer simulations which determined the direction of motion of one particle for various initial conditions. Fig. 3 shows the respective trajectories for the movement in both directions and the separatrix plane. We can conclude 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. This conclusion will be of importance when discussing the current reversal in a ratchet potential in Sect. 4. In particular, in Sect. 4.1 we will investigate the existence of critical conversion rates \( d_2 \) in more detail by comparing analytical results and computer simulations.

### 3.2 Deterministic vs. Stochastic Motion

In the following, the motion of an ensemble of \( N \) pumped Brownian particles in a ratchet potential, Eq. (23), is investigated both for the deterministic and the stochastic case. For the computer simulations, we have assumed that the start locations of the particles are equally distributed over the first period of the potential, \( \{0, L\} \). We note, that in the computer simulations always the complete set of equations (10) for the particles is solved.

In the deterministic case, the direction of motion and the velocity at any time \( t \) are mainly determined by the initial conditions. Provided a sufficient supply of energy, particles with an initial position between \( \{0, b\} \), which initially feel a force into the negative direction, most likely move with a negative velocity, whereas particles with an initial position between \( \{b, L\} \) most likely move into the positive direction. For parameter values which allow the existence of two unbound attractors (cf. also Fig. 2c), Fig. 4 shows the final distribution of the velocities in the deterministic case.

We see two main currents of particles occurring, with a positive and a negative velocity. The net current, however, has a positive direction, since most of the particles start with the matching initial condition. The time dependence of the averages is shown in the first part of Fig. 5 for \( t \leq 2.000 \). The long-term oscillations in the average velocity and the average energy depot result from the superposition of the velocities, which are sharply peaked around the two dominating values, shown in Fig. 4.

In order to demonstrate the influence of fluctuations on the mean values \( \langle x \rangle, \langle v \rangle, \langle e \rangle \), we add a stochastic force with \( D > 0 \) to the simulation of the ensemble of pumped Brownian particles.
shown in Fig. 5 at $t = 2.000$. Hence, the second part of Fig. 5 demonstrates the changes after the stochastic force is switched on. The simulations show that the current changes its direction when noise is present. Different from the deterministic case, Fig. 4, the related velocity distribution in the stochastic case now approaches an one peak distribution, shown in Fig. 6. Hence, stochastic effects are able to stabilize the motion in the vicinity of the unbound attractor which corresponds to the negative current, while they destabilize the motion in the vicinity of the unbound attractor corresponding to the positive current, both shown in Fig. 2c.

A similar situation can be also observed when the motion of the particles is less damped (cf. Fig. 7). For this case, we clearly see both the mean velocity and the mean energy depot approaching constant values, instead of oscillating. Further, the time scale of the relaxation into the stationary values decreases with the intensity of the stochastic force.

The related velocity distribution of the particles is plotted for different intensities of the stochastic force in Fig. 8. For $D = 0$, there are two sharp peaks at positive values for the speed and one peak for negative values, hence, the average current is positive. The three maxima correspond to the stationary velocities in the deterministic case. For $D = 0.001$, the distribution of positive velocities is declining, since most of the particles already move with a negative velocity, and for $D = 0.01$ after the same time all particles have a negative velocity. Further, the velocity distribution becomes more broaden in the presence of noise.

As a result of the computer simulations presented in this section, we find that an ensemble of pumped Brownian particles moving in a ratchet potential is able to produce a directed net current. In the deterministic case, we find two currents into opposite directions related to a sharply peaked bimodal velocity distribution, and the direction of the resulting net current is determined by the initial conditions of the majority of the particles. In the stochastic case, however, we find only a broad and symmetric unimodal velocity distribution, resulting in a stronger net current. The direction of this net current is opposite to the deterministic case and points into the negative $x$-direction. This reversal will be discussed in more detail in the next section.

4 Investigation of the Current Reversal

4.1 Dependence on Energy Conversion and Noise

The previous computer simulations revealed the dependence of the net current on the initial conditions and on the influence of the stochastic force. Since all particles have started in the first period of the ratchet potential, the existence of periodic stationary solutions, $v_0(x) = v_0(x \pm L)$, requires that the particles are able to escape from the potential well. Hence, they must be able to move “uphill” on one or both flanks of the ratchet potential, in order to obtain a net current. In the phase
space, this corresponds to the formation of unbound attractors corresponding to directed motion in the ratchet potential. This, in turn, would require a supercritical supply of energy for the pumped Brownian particles to move in the active or “high velocity” mode, as already mentioned in Sect. 2.

Eq. (20) provides a necessary condition for a stable uphill motion on a single flank in terms of a critical conversion rate $d_2^{crit}$. In order to demonstrate the applicability of Eq. (20) for the ratchet potential, we have investigated the dependence of the net current, expressed by the mean velocity $\langle v \rangle$, on the conversion rate, $d_2$. The deterministic motion is for the overdamped case discussed in [19], here we concentrate on the less damped case and discuss both the deterministic and the stochastic motion. The results of computer simulations are shown in Fig. 9.

For the deterministic motion, we see the existence of two different critical values for the parameter $d_2$, which correspond to the onset of a negative net current at $d_2^{crit1}$ and a positive net current at $d_2^{crit2}$. 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. Consequently, after the initial downhill motion, the particles perform a localized motion (oscillation) within the potential well (cf. also Fig. 2a) and no current occurs. The amplitude of these oscillations depends on the conversion rate $d_2$. In the limit of vanishing energy conversion the motion of the particles comes to rest in the minima of the ratchet potential.

With an increasing value of $d_2$, we see the occurrence 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, which, in our example, is the one with $F = 7/8$ (cf. Fig. 1). If we insert this value for $F$ into the critical condition, Eq. (20), a value $d_2^{crit1} = 1.03$ is obtained, which agrees with the onset of the negative current in the deterministic computer simulations, Fig. 9.

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 the same does not necessarily apply for the steeper slope. Hence, particles which start on the lower slope with a positive velocity, cannot continue their motion into the positive direction since they are not able to climb up the steeper slope. Consequently, they turn their direction on the steeper slope, then move downhill driven by the force into the negative direction, and continue to move into the negative direction while climbing up the lower slope. Therefore, for values of the conversion rate between $d_2^{crit1}$ and $d_2^{crit2}$, we only have an unimodal distribution of the velocity, and only one unbound attractor exists as shown in Fig. 2b.

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. In our example, the steeper slope corresponds to the force $F = -7/4$ (cf. Fig. 1) which yields a critical value $d_2^{crit1} = 11.3$, obtained by means of Eq. (20). This result agrees with the onset of the positive current in the computer simulations, Fig. 9. For $d_2 > d_2^{crit2}$, we have a bimodal velocity distribution in the deterministic case, as also shown in the top part of Fig. 8. This corresponds to the existence of two unbound attractors as shown in Fig. 2c. For equally distributed
initial positions of the particles, the net current which results from the average of the two main currents has a positive direction in the deterministic case, because most of the particles start into a positive direction, as discussed above.

Let us now turn to the stochastic case. In Sect. 3, we have already shown that the influence of a stochastic force may lead to a current reversal. In the deterministic case, the particles will keep their direction determined by the initial conditions provided the energy supply allows them to move “uphill”, which is the case for \( d_2 > d_2^{crit} \). In the stochastic case, however, the initial conditions will be “forgotten” after a short time, hence due to stochastic influences, the particle’s “uphill” motion along the steeper flank will soon turn into a “downhill” motion. This motion into the negative direction will be most likely kept because less energy is needed. Thus, the stochastic fluctuations reveal the instability of an “uphill” motion along the steeper slope.

For a comparison with the deterministic case, Fig. 9 shows the average velocity also for the stochastic case. Here, the net current is always negative in agreement with the explanation above. This holds even if the supercritical supply of energy, expressed by the conversion parameter, \( d_2 > d_2^{crit} \), would allow a deterministic motion into the positive direction (cf. the dashed line in Fig. 9). In addition, we find a very small positive net current in the range of small \( d_2 \) (cf. the insert in Fig. 9). Whereas in the deterministic case, for the same values of \( d_2 \) no net current at all is obtained, the fluctuations in the stochastic case 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 \( d_2 = 1.0 \) for the less damped case. As Fig. 9 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. 10 shows, there is a critical strength of the stochastic force, \( D^{crit}(d_2 = 1.0) \approx 10^{-4} \), 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.

### 4.2 Dependence on Potential Asymmetry

We conclude our results by investigating the influence of the slope on the establishment of a positive or negative net current. With a fixed height of the potential barrier \( U_0 \), and a fixed length \( L \), the ratio of the two different slopes is described by the asymmetry parameter \( a \) of the ratchet potential, Eq. (24). In the deterministic case, the occurrence of a current in the ratchet potential depends on the critical supply of energy, described by Eq. (20). In order to obtain the critical value for the asymmetry of the potential, we replace the force \( F \) in Eq. (20) by the parameter \( a \), Eq. (24). In our
example, the flank $l_1$ of the potential has the steeper slope, so the critical condition is determined by $F_1 = U_0/L (1 + a)$. As the result, we have found [19]:

$$a_{\text{crit}} = \frac{L}{U_0} \left[ -\frac{\gamma_0}{2} d_2^{-1/3} + \sqrt{\frac{\gamma_0^2}{4} d_2^{-2/3} + q_0 d_2^{1/3}} \right]^{3/2} - 1$$

$a_{\text{crit}} \geq 1$ gives the critical value for the asymmetry, which may result in a reversal of the net current in the deterministic case.

Fig. 11 shows the average velocity, $\langle v \rangle$, dependent on the asymmetry parameter, $a$. The simulations have been carried out for different values of the stochastic force in the overdamped case, for a fixed value $d_2 = 10$. In particular, the top part of Fig. 11 also includes the curve for $D = 0$. As we see in the deterministic case, for $a > a_{\text{crit}}$ the flank $l_1$ is too steep for the particles, therefore only a negative current can occur. For $1 < a < a_{\text{crit}}$, however, the particles are able to move uphill either flank. Hence, also a positive net current can establish.

As long as the stochastic forces are below a critical value, $D < D_{\text{crit}}$, which is about $D_{\text{crit}} (d_2 = 10) \simeq 0.02$, the curves for the stochastic case are not very different from the deterministic one, as shown in the top part of Fig. 11. Hence, the above conclusions about the current reversal in the deterministic case apply. However, for $D > D_{\text{crit}}$ (cf. the bottom part of Fig. 11) we do not find a critical asymmetry $a_{\text{crit}}$ for a current reversal. Instead, the net current keeps its positive (for $a < 1$) or negative (for $a > 1$) direction for any value of $a < 1$ or $a > 1$, respectively.

The bottom part of Fig. 11 further indicates the existence of an optimal strength of the stochastic force, again. Similar to the investigations in Fig. 10, we find that an increase in $D$ does not necessarily results in a increase of the amount of the net current. In fact, the maximum value of $|\langle v \rangle|$ is smaller for $D = 0.1$ than for $D = 0.05$, which indicates an optimal strength of the stochastic force, $D_{\text{opt}}$, between 0.05 and 0.1 for the considered set of parameters.

We note that the values for both the critical strength, $D_{\text{crit}}$, and the optimal strength, $D_{\text{opt}}$, of the stochastic force depend on the value of the conversion parameter, $d_2$, as a comparison of Fig. 10 and Fig. 11 shows. Further, these values may be also functions of the other parameters, such as $q_0$, $\gamma_0$, and therefore differ for the strongly overdamped and the less damped case.

5 Conclusions

In Sects. 3 and 4, we have shown by means of computer simulations, that an ensemble of pumped Brownian particles moving in a ratchet potential can produce a directed net current. Hence, by means of an appropriate asymmetric potential and an additional mechanism to drive the system into non-equilibrium, we are able to convert the genuinely non-directed Brownian motion into directed motion. In this respect, our result agrees with the conclusions of other physical ratchet models.
which have been proposed to reveal the microscopic mechanisms resulting in directed movement. In order to point out some differences to our model, we first need to summarize the basic principles. Ratchet models which describe the directed transport of particles, are usually based on three ingredients: (i) an asymmetric periodic potential, known as ratchet potential, Eq. (23), Fig. 1, which lacks the reflection symmetry, (ii) stochastic forces $\xi(t)$, i.e. the influence of noise resulting from thermal fluctuations on the microscale, and (iii) additional correlations, which push the system out of thermodynamic equilibrium. For the latter one, different assumptions can be made. In the example of the flashing ratchet, the correlations result from an fluctuating energy profile. In the overdamped limit, the dynamics of a Brownian particle can then be described by the equation of motion:

$$\frac{dx}{dt} = -\zeta(t) \frac{\partial U(x)}{\partial x} + \sqrt{2D} \xi(t)$$

The nonequilibrium forcing $\zeta(t)$ which governs the time dependent change of the potential, can be either considered as a periodic, deterministic modulation with period $\tau$, $\zeta(t) \to F(t) = F(t + \tau)$, or as a stochastic non-white process $\zeta(t)$. In the special case where $\zeta(t)$ or $F(t)$ have only the values $\{0, 1\}$, the periodic potential is switched ON and OFF.

In another class of ratchet models, the additional correlations result from spatially uniform forces of temporal or statistical zero average. In the example of the rocking ratchet, the particles are subject to a spatially uniform time-periodic deterministic force $F(t) = F(t + \tau)$, for instance:

$$\frac{dx}{dt} = -\frac{\partial U(x)}{\partial x} - A \cos\left(\frac{2\pi t}{\tau}\right) + \sqrt{2D} \xi(t)$$

Here, the potential $U_s(x, t) = U(x) + A x \cos(\Omega t)$ is periodically rocked. If the value of $A$ is adjusted properly, in the deterministic case a net current of particles into the direction of the lower slope can be observed, while the movement into the direction of the steeper slope is still blocked. However, a consideration of stochastic influences results in a current reversal for a certain range of the parameters $A$ and $D$ [20]. Then, the net current occurs again in the direction of the steeper slope. Because this phenomenon depends also on the mass of the particles, it can be used for mass separation [21].

Another example of the same class, the correlation ratchet [3–5], is also driven by a spatially uniform, but stochastic force, $\zeta(t)$. Here, the equation for the overdamped motion reads for instance:

$$\frac{dx}{dt} = -\frac{\partial U(x)}{\partial x} + \zeta(t) + \sqrt{2D} \xi(t)$$

where $\zeta(t)$ is a time correlated (colored) noise of zero average. As a third example, the diffusion ratchet [22] is driven by a spatially uniform, time-periodic diffusion coefficient $D(t) = D(t + \tau)$, which may result e.g. from an oscillating temperature. In the overdamped limit, the equation of
motion reads for example:

\[ \frac{dx}{dt} = -\frac{\partial U(x)}{\partial x} + \zeta(t) + \left[1 + A \sin(\Omega t)\right] \sqrt{2D} \xi(t) \]  (29)

Inspite of the different ways to introduce additional correlations, all these models have in common to transfer the undirected motion of Brownian particles into directed motion, hence, the term Brownian rectifiers [8] has been established.

As we have shown in this paper, our own model can also serve for this purpose. For a comparison with the models above, we rewrite Eq. (16) for the overdamped motion of the Brownian particles with internal energy depot in a more general way:

\[ \frac{dx}{dt} = -f(t) \frac{\partial U(x)}{\partial x} + C f(t) \sqrt{2D} \xi_i(t) ; \quad f(t) = \frac{1}{\gamma_0 - d_2 e(t)} \]  (30)

In Eq. (30), the prefactor \( f(t) \) appears twice, up to a constant \( C \): it changes both the influence of the ratchet potential, and the magnitude of the diffusion coefficient. In this respect, our model is between a flashing ratchet model, Eq. (26), and a diffusion ratchet model, Eq. (29).

\( f(t) \) is in general a time dependent function, because of \( e(t) \). In the limit of a stationary approximation, \( e(t) \to e_0 \), Eq. (11), we found [19] that \( f(t) \) may switch between two constant values \( f_1(x) > 0, f_2(x) < 0 \):

\[ f_i(x) = \frac{1}{2\gamma_0 F_i} \left( F_i \pm \sqrt{F_i^2 + 4q_0\gamma_0} \right) \]  (31)

dependent on the moving direction and the flank, the particle is moving on. Hence, the function \( f(t) \) does not represent a spatially uniform force. However, it has been shown in [19], that for the stationary approximation \( \langle \gamma_0 - d_2 e_0 \rangle \tau = 0 \) holds, i.e. the force is of zero average with respect to one period, \( \tau \). Hence, we conclude that the mechanism of motion which Eq. (16) is based on, should be different from the previous mechanisms which originate directed motion in a ratchet potential.

Finally, we note that the model of active Brownian particles with internal energy depot is not restricted to ratchet systems. In a general sense, these particles can be described as Brownian machines or molecular motors which convert chemical energy into mechanical motion. While different ideas for Brownian machines have been suggested [9–11], our model aims to add a new perspective to this problem. The ability of the particles to take up energy from the environment, to store it in an internal depot and to convert internal energy to perform different activities, may open the door to a more refined description of microbiological processes based on physical principles.

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**Figures**

![Figure 1: Sketch of the asymmetric potential $U(x)$ (eq. (23)). For the computer simulations, the following values are used: $b=4$, $L=12$, $U_0 = 7$ in arbitrary units.](image-url)
Figure 2: Phase-space trajectories of particles starting with different initial conditions, for three different values of the conversion parameter $d_2$: (a: top) $d_2 = 1$, (b: middle) $d_2 = 4$, (c: bottom) $d_2 = 14$. Other parameters: $q_0 = 1$, $c = 0.1$, $\gamma_0 = 0.2$. The dashed-dotted lines in the middle and bottom part show the unbound attractor of the delocalized motion which is obtained in the long-time limit.
Figure 3: Separatrix and asymptotic trajectories in the \{x, v, e\} phase space. Parameters see Fig. 2c. In order to obtain the separatrix in Fig. 3, we have computed the velocity \(v_0\) for given values of \(x_0\) and \(e_0\) (in steps of 0.01) using the Newton iteration method with a accuracy of 0.0001.

Figure 4: Distribution of the final velocity \(v_e\) after \(t = 2.000\) simulation steps (averaged for 10.000 particles). The initial locations of the particles are equally distributed over the first period of the ratchet potential \(\{0, L\}\). Parameters: \(q_0 = 10, \gamma = 20, e = 0.01, d_2 = 10\) (strongly damped case).
Figure 5: Averaged location $\langle x \rangle$, velocity $\langle v \rangle$ and energy depot $\langle e \rangle$ versus time $t$ for 10,000 particles. The stochastic force $D = 0.01$ is switched on at $t = 2.000$. Parameters see Fig. 4.

Figure 6: Distribution of velocity $v$ for the simulation of Fig. 5 at time $t = 4.000$, which means 2,000 simulation steps after the stochastic force was switched on.
Figure 7: Averaged location $\langle x \rangle$, velocity $\langle v \rangle$ and energy depot $\langle e \rangle$ versus time $t$ for 10,000 particles. The stochastic force, either $D = 0.01$ or $D = 0.001$, is switched on at $t = 250$. Parameters: $q_0 = 1.0, \gamma = 0.2, c = 0.1, d_2 = 14.0$ (less damped case).
Figure 8: Distribution of velocity $v$ for the simulation of Fig. 7. (top) $D = 0.0$ ($t = 250$), (middle) $D = 0.001$ ($t = 500$), (bottom) $D = 0.01$ ($t = 500$). The stochastic force is switched on at $t = 250$. 
Figure 9: 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. (◇) stochastic case ($D = 0.1$), (○) deterministic case ($D = 0$), for the other parameters see Fig. 7.

Figure 10: 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.
Figure 11: Average velocity $\langle v \rangle$ vs. asymmetry parameter $a$, Eq. (24). The data points are obtained from simulations of 10,000 particles with arbitrary initial positions in the first period of the ratchet potential. (top) subcritical stochastic force: (○) $D = 0$ (-----), (◇) $D = 0.001$ (---), (□) $D = 0.01$ (···), (bottom) supercritical stochastic force: (△) $D = 0.05$ (-----), (▽) $D = 0.1$ (---). $d_2 = 10$, for the other parameters see Fig. 4.