Complex Motion of Brownian Particles with Energy Depots

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We investigate the motion of Brownian particles which have the ability to take up energy from the environment, to store it in an internal depot, and to convert internal energy into kinetic energy. The resulting Langevin equation includes an additional acceleration term. The motion of the Brownian particles in a parabolic potential is discussed for two different cases: (i) continuous take-up of energy and (ii) take-up of energy at localized sources. If the take-up of energy is above a critical value, we found a limit-cycle motion of the particles, which, in case (ii), can be interrupted by stochastic influences. Including reflecting obstacles, we found for the deterministic case a chaotic motion of the particle. [S0031-9007(98)06328-5]

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Active motion is based on energy consumption. For biological systems, an external supply of energy is crucial, e.g., to maintain metabolism and to perform movement [1]. For a spatially inhomogeneous supply of energy, the organism needs to store energy internally, in order to overcome periods of starvation, e.g., during the search for new sources. But even provided the homogeneous supply of energy, the organism needs to convert the energy taken up from the environment into kinetic energy. Dependent on the level of biological organization, the take-up, storage, and conversion of energy is a rather complex process.

In the following, we consider the motion of microscopic biological objects, such as cells or bacteria, which can be sufficiently described by a Langevin dynamics. Stochastic differential equations have long been used to describe the motion of organisms [2,3]. In order to derive a simplified model of active biological motion, we study Brownian particles with 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:

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

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 S and a δ-correlated time dependence

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

Recently, Brownian motion models attracted much attention for describing nonequilibrium transport on the microscale [4]. In addition to the dynamics described above, the Brownian particles discussed here are active particles [5] to the effect that they have the ability to take up energy from the environment and to store it in an internal depot, which is considered a new element of the model. Further, the particles are able to convert internal energy into kinetic energy. Considering also internal dissipation, the resulting balance equation for the internal energy depot, e, of an active particle is given by

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

$q(\boldsymbol{r})$ is the space-dependent take-up of energy and c describes the internal dissipation assumed to be proportional to the depot energy. $d(\boldsymbol{v})$ is the rate of conversion of internal into kinetic energy which should be a function of the actual velocity of the particle. A simple ansatz for $d(\boldsymbol{v})$ reads: $d(\boldsymbol{v}) = d_2 v^2$; $d_2 > 0$. The total energy of the active particle at time t is given by

$$E(t) = E_0(t) + e(t)\,,$$
$$E_0(t) = \frac{m}{2}\, v^2 + U(\boldsymbol{r})\,. \tag{4}$$

$E_0(t)$ is the mechanical energy of the active particle moving in the potential $U(\boldsymbol{r})$, which can be (i) increased by the conversion of depot energy into kinetic energy, (ii) decreased by the friction of the moving particle resulting in dissipation of energy. Hence, the balance equation for the mechanical energy reads

$$\frac{d}{dt}\, E_0(t) = (d_2 e(t) - \gamma_0)\, v^2. \tag{5}$$

Combining Eqs. (4) and (5), we can rewrite Eq. (5) in a more explicit form:

$$m\dot{\boldsymbol{r}}\ddot{\boldsymbol{r}} + \dot{\boldsymbol{r}}\, \nabla U(\boldsymbol{r}) = [d_2 e(t) - \gamma_0]\, \dot{r}^2. \tag{6}$$

Based on Eq. (6), we postulate a stochastic equation of motion for the active Brownian particles which is consistent with the Langevin equation (1):

$$m\dot{\boldsymbol{v}} + \gamma_0 \boldsymbol{v} + \nabla U(\boldsymbol{r}) = d_2 e(t) \boldsymbol{v} + \mathcal{F}(t)\,. \tag{7}$$

Compared to previous investigations [6] the first term of the right-hand side of Eq. (7) is the essential new element in this paper, reflecting the influence of the internal energy depot to the motion of Brownian particles. It describes the acceleration in the direction of movement, $\boldsymbol{e}_v = \boldsymbol{v}/v$, due to the conversion of internal into kinetic energy. Using the fluctuation-dissipation theorem, we

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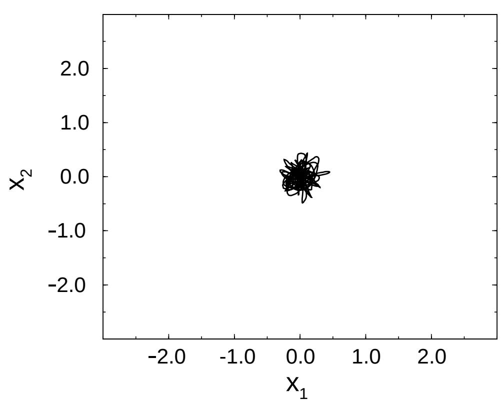
assume that the loss of energy resulting from friction, and the gain of energy resulting from the stochastic force, are compensated in the average, and S can be expressed as $S = k_B T \gamma_0$. The balance equation for the mechanical energy, Eq. (5), has then for the stochastic case to be modified to

$$\frac{d}{dt}\left[\frac{1}{2}m\dot{r}^2 + U(\boldsymbol{r})\right] = d_2 e(t)\dot{r}^2. \tag{8}$$

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

$$U(x_1, x_2) = \frac{a}{2}(x_1^2 + x_2^2). \tag{9}$$

This potential originates a force directed to the minimum of the potential; however, the random force in Eq. (7) keeps the particle moving, even without the take-up of energy (Fig. 1, top). Going over from the simple Brownian motion to the active Brownian motion, in a first assumption the take-up of energy, $q(\boldsymbol{r})$ is considered as constant in space: $q(x_1, x_2) = q_0$. Figure 1 (bottom) demonstrates that the take-up of energy and its conversion into kinetic energy allows the particle to reach out farther, moving on a stochastic limit cycle, if some critical conditions are satisfied.



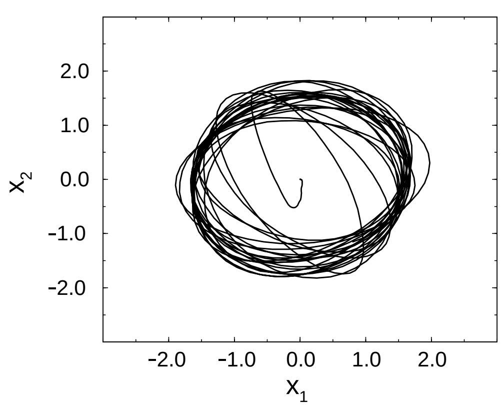


FIG. 1. Stochastic motion of an active Brownian particle in a parabolic potential, Eq. (9) ($a = 2$). (top) $q = 0$ (simple Brownian motion); (bottom) $q_0 = 1.0$. Other parameters: $\gamma_0 = 0.2$ $d_2 = 1.0$, $c = 0.1$, $S = 0.01$. Initial conditions: $(x_1, x_2) = (0, 0)$, $(v_1, v_2) = (0, 0)$, $e(0) = 0$.

In order to derive these critical parameters, we consider the active Brownian particle as a micromotor. Molecular motors based on Brownian motion have been recently introduced [7]. For the Brownian particle with energy depot, the efficiency ratio is defined as

$$\sigma = \frac{dE_{\text{out}}/dt}{dE_{\text{in}}/dt}. \tag{10}$$

The input of energy per time interval, dE_{in}/dt, is given by the take-up, q_0, while the output, dE_{out}/dt, is defined as the amount of mechanical energy available from the micromotor, Eq. (8). The term $d_2 e(t) v^2$ can be approximated using the following assumptions:

(i) Compared to the time scale of motion, the internal energy depot reaches fast a quasistationary equilibrium. With $\dot{e}(t) = 0$, we find

$$e = \frac{q_0}{c + d_2 v^2}. \tag{11}$$

(ii) The velocity, $\boldsymbol{v}$, can be approximated by the stationary velocity, $\boldsymbol{v}_0$ obtained in the deterministic limit [8]:

$$v_0^2 = (v_1^2 + v_2^2) = \frac{q_0}{\gamma_0} - \frac{c}{d_2}. \tag{12}$$

With these assumptions, σ, Eq. (10), can be expressed as follows:

$$\sigma = 1 - \frac{c\ \gamma_0}{d_2\ q_0}. \tag{13}$$

The efficiency ratio, which is equal to 1 only in the ideal case, is decreased by dissipative processes, like friction (γ_0) and internal dissipation (c). Moreover, σ is larger than zero only if the take-up of energy is above the critical value:

$$q_0 > q_0^{\text{crit}} = \frac{\gamma_0 c}{d_2}. \tag{14}$$

Provided a supercritical supply of energy, the particle periodically moves on the stochastic limit cycle shown in Fig. 1 (bottom).

In a second example, we discuss the case that the energy sources are localized in space. Then, the internal depot of the active Brownian particles can be refilled only in a restricted area. This is reflected in a space dependence of the energy influx $q(\boldsymbol{r})$, for example:

$$q(x_1, x_2) = \begin{cases} q_0, & \text{if } [(x_1 - b_1)^2 + (x_2 - b_2)^2] \leq R^2, \\ 0, & \text{else}. \end{cases} \tag{15}$$

Here, the 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 is empty and

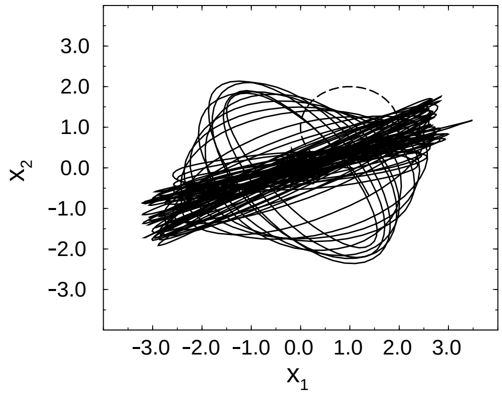


FIG. 2. Trajectories in the x_1, x_2 space for the stochastic motion of an active Brownian particle in a parabolic potential, Eq. (9). $(a = 2)$ The circle [coordinates (1,1), radius $R = 1$] indicates the area of energy supply, Eq. (15). Parameters: $q_0 = 10.0$, $\gamma_0 = 0.2$ $d_2 = 0.1$, $c = 0.01$, $S = 0.01$. Initial conditions: $(x_1, x_2) = (0, 0)$, $(v_1, v_2) = (0, 0)$, $e(0) = 0$).

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 particle's motility, as presented in Fig. 2. Most likely, the motion into the energy area becomes accelerated, 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, as shown in Fig. 3. Then the active particle, with an empty internal depot, moves again like a simple Brownian particle, until a new cycle starts. This way the particle motion is of intermittent type [9]. We found that the trajectories eventually cover the whole area inside certain boundaries; however, during an oscillation period the direction is most likely kept.

Every new cycle starts with a burst of energy in the depot, which can be understood on the basis of Eq. (3). At the start of each cycle, e is small and de/dt is very large, thus a burst follows, which is used for the acceleration of the particle. However, an increase in $d_2 v^2 e$ makes the last term in Eq. (3) more negative and the growth of e is more rapidly cut off. This is, for the beginning of the first cycle in Fig. 3, shown in more detail in Fig. 4, which also clearly indicates the oscillations. The transition time into the oscillation regime, as well as the duration of the oscillatory cycle depend remarkably on the conversion parameter, d_2. The bottom part of Fig. 4, to be compared with the part above, indicates that an increase in d_2 reduces the amount of the bursts and abridges the cycle. For a larger d_2, more depot energy is converted into kinetic energy. Hence, with less energy in stock the particle's motion is more susceptible to become Brownian motion again, if stochastic influences prevent the particle from returning to the source in time.

Real biological motion occurs in complicated landscapes which typically not only contain localized areas of energy supply, but also obstacles. This may lead to a rather complex active motion. In our simple model, the existence an of obstacle can be implemented in the

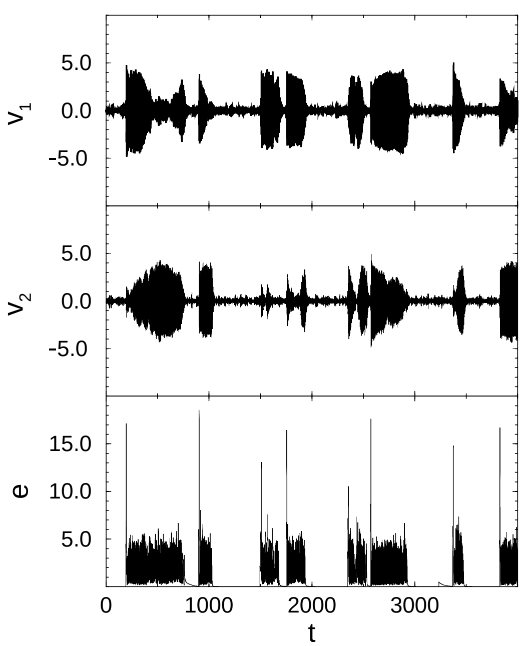


FIG. 3. Velocities in the x_1, x_2 space and internal energy depot vs time for the stochastic motion, shown in Fig. 2.

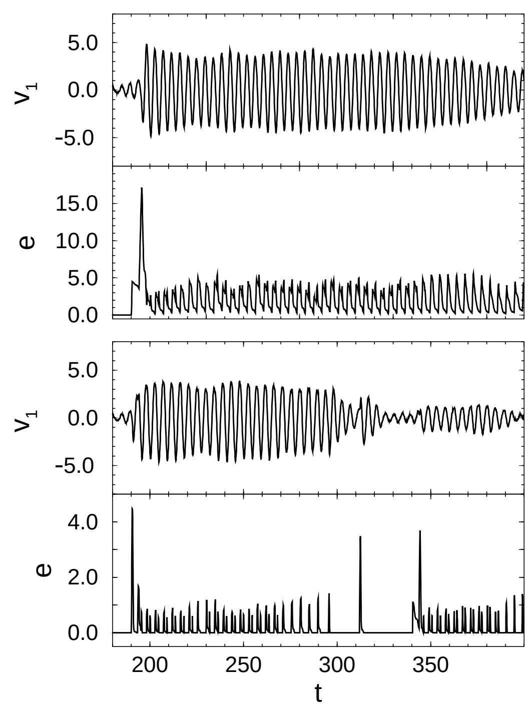


FIG. 4. Velocity v_1 and internal energy depot e vs time for two different values of d_2: (top) $d_2 = 0.1$ (enlarged part of Fig. 3), (bottom) $d_2 = 1.0$. (Other parameters, see Fig. 2.)

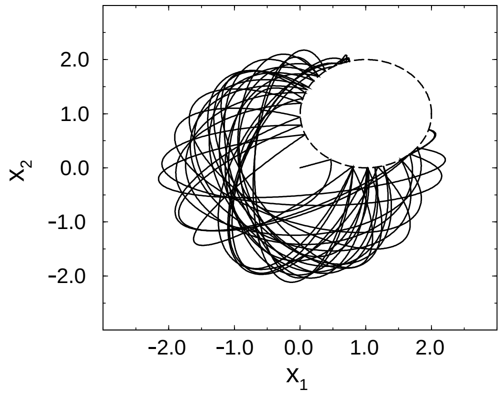


FIG. 5. Trajectories in the x_1, x_2 space for the *deterministic* motion of an active Brownian particle in a parabolic potential, Eq. (16), $(a = 2)$ where the circle [coordinates (1,1), radius $R = 1$] indicates the reflecting obstacle. Parameters: $q_0 = 1.0$, $\gamma_0 = 0.2$ $d_2 = 1.0$, $c = 0.1$. Initial conditions: $(x_1, x_2) = (0,0)$, $(v_1, v_2) = (1.0, 0.33)$, $e(0) = 0$.

potential U [Eq. (9)], for example:

$$U(x_1, x_2) = \frac{a}{2}(x_1^2 + x_2^2) + U_0\,\Theta[R^2 - (x_1 - b_1)^2 - (x_2 - b_2)^2], \quad (16)$$

with $U_0 \to \infty$ and Θ being the Heaviside function:

$$\Theta[R^2 - r^2] = \begin{cases} 1, & \text{if } r^2 \leq R^2, \\ 0, & \text{else.} \end{cases} \quad (17)$$

Equation (17) models an obstacle centered around the point (b_1, b_2) which has the form of a hard core with the radius R. If the particle hits the obstacle, it is simply reflected at the boundary, R. We want to consider here again a continuous supply of energy, $q(x_1, x_2) = q_0$, but only a deterministic motion of the particle, i.e., $S = 0$. Then, the initial conditions, $\boldsymbol{v} \neq 0$, determine whether the particle can start its motion and will hit the obstacle, or not. As Fig. 5 shows, the existence of reflecting obstacles results in a complex motion of the active particle, even in the deterministic case.

In the case of pure Hamiltonian mechanics, there is an analogy to the Sinai–billiard, where Hamiltonian chaos has been found [10,11]. In our model, the situation is different, since we do not have energy conservation, but energy dissipation on one hand, and the influx of energy on the other hand. In order to decide whether the motion shown in Fig. 5 is chaotic, we have calculated the Lyapunov exponent, λ, which characterizes how a small perturbation of the trajectory $\boldsymbol{r}$, $\Delta\boldsymbol{r}(t_0) = \boldsymbol{r}(t_0) - \boldsymbol{r}'(t_0)$, evolves in the course of time, $t > t_0$. The motion becomes asymptotically unstable, if $\lambda > 0$. Using standard methods described, e.g., in [12], we found, for the parameters used in Fig. 5, the largest Lyapunov exponent as $\lambda = 0.17$. This indicates a chaotic motion of the active particle in the phase space $\Gamma = \{x_1, x_2, v_1, v_2, e\}$. Hence, we conclude that for the motion of Brownian particles with energy depots reflecting obstacles have an effect similar to stochastic influences (external noise), both producing interesting forms of complex motion. The examples discussed above can be generalized by considering different obstacles, or different localized energy sources, which also allows one to draw analogies to the search for food in biological systems.

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