Frank Schweitzer: Active Motion of Brownian Particles
in: *Stochastic Processes in Physics, Chemistry and Biology* (Eds. J. A. Freund, T. Pöschel)
Lecture Notes in Physics vol. 557, Springer, Berlin 2000, pp. 97–106

Active Motion of Brownian Particles

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Abstract

We investigate the dynamics of Brownian particles which are active in the sense that they take up energy from the environment, which can be stored in a internal energy depot and used for different activities. As one example, we consider the generation of a self-consistent field, which in turn affects the movement of the particles. The dynamics can in this case be described by coupled reaction-diffusion equations, but will be more efficiently simulated by means of Langevin equations for the active particles. As another example, we discuss the active motion of Brownian particles which can be described by a non-linear, velocity-dependent friction function. Provided a supercritical supply of energy, the active particles are able to perform non-trivial motion, such as "uphill" motion against the direction of an external force, or motion on a stochastic limit cycle.

1 Simulation of Reaction-Diffusion Systems

Reaction-diffusion systems are known to exhibit a large variety of fascinating patterns. Among the prominent examples are spiral patterns in the Belousov–Zhabotinsky reaction, or patterns on sea shells or mammalian coats. Despite their very different appearence, the basic dynamics of these patterns can in many cases be described by a set of coupled reaction-diffusion equations. For the case of two distributed components C_m and C_n with the spatio-temporal densities $m(\vec{r},t)$ and $m(\vec{r},t)$, they are in general of the form:

$$\frac{\partial m(\vec{r},t)}{\partial t} = \mathcal{F}(m,n) + D_m \Delta m(\vec{r},t) \quad (1)$$

$$\frac{\partial n(\vec{r},t)}{\partial t} = \mathcal{G}(m,n) + D_n \Delta n(\vec{r},t) \quad (2)$$

Here, the last term of both equations describes the spatial diffusion of the different components, while the functions $\mathcal{F}(m,n)$ and $\mathcal{G}(m,n)$ describe the interaction between the two components. Let

us, as one example, assume that the first component, C_m, will be produced by the second one at a spatially constant rate s and that its concentration further decays at a contant rate, k_m. Then, the reaction function $\mathcal{F}(m,n)$ reads:

$$\mathcal{F}(m,n) = s\, n(\vec{r},t) \;-\; k_m\, m(\vec{r},t) \tag{3}$$

The particles of the second component, C_n, on the other hand, should exist at a constant number N, i.e.

$$N = \int_A n(\vec{r},t)\, dr = \text{const.} \tag{4}$$

and will be only affected by the *gradient* of the density $m(\vec{r},t)$ in the following manner:

$$\mathcal{G}(m,n) = -\frac{\partial}{\partial r}\left[\alpha \frac{\partial m(\vec{r},t)}{\partial r}\, n(\vec{r},t)\right] \tag{5}$$

With eq. (5), eq. (2) for the second component becomes in fact a Fokker–Planck equation, where $\mathcal{G}(m,n)$ denotes the drift term. If $m(\vec{r},t)$ in eq. (5) would be replaced by a time-independent function $U(\vec{r})$, for instance, this term would describe the motion of the C_n particles in the external potential $U(\vec{r})$. But in this case, the "potential" is also created by the C_n particles according to eq. (3) and is therefore denoted as a self-consistent field. Here, α denotes the "strength" of the response to the gradient of the field.

The non-linear feedback between the particles with density $n(\vec{r},t)$ and the self-consistent field $m(\vec{r},t)$, may result in a spatial structure formation, that has been investigated by Schimansky-Geier *et al.* in different variants [16, 17]. A particular application of this model may describe the aggregation of larvae and other biological species (denoted by C_n) which communicate via a chemical field (denoted by $m(\vec{r},t)$), using chemotactic response [21].

A conventional way to investigate this spatio-temporal process would be the integration of the two coupled differential eqs. (1), (2), with respect to eqs. (3), (5). The time step required for the integration, is mainly determined by the nonlinearities of the equations. Suppose that $n(\vec{r},t)$ and $m(\vec{r},t)$ are of the same order, then the allowed time step Δt should be less than:

$$\Delta t < \left(\alpha \left|\frac{\partial n(\vec{r},t)}{\partial \vec{r}} \frac{\partial m(\vec{r},t)}{\partial \vec{r}}\right|\right)^{-1} \sim \left(\alpha \left[\frac{\partial m(\vec{r},t)}{\partial \vec{r}}\right]^2\right)^{-1} \tag{6}$$

i.e. it should decrease according to the *square* of $\vec{\nabla} m$. In the presence of strong gradients, this could be sometimes rather decelerating. Therefore, it would be convenient to find a more efficient simulation method.

An alternative, particle-based approach, which may result in a much faster computer simulation, is based on the correspondence between the Fokker–Planck equation, (2), (5), and the overdamped Langevin equation,

$$\frac{d\vec{r}_i}{dt} = \alpha \left.\frac{\partial m(\vec{r},t)}{\partial \vec{r}}\right|_{\vec{r}_i} + \sqrt{2\, D_n}\, \vec{\xi}_i(t) \tag{7}$$

The second term of eq. (7) results from a stochastic force, where the random function $\vec{\xi}_i(t)$ is assumed to be Gaussian white noise, $\left\langle \vec{\xi}_i(t) \right\rangle = 0$, $\left\langle \vec{\xi}_i(t)\, \vec{\xi}_j(t') \right\rangle = \delta_{ij}\, \delta(t-t')$. While eqs. (2), (5) refer to the particle density $n(\vec{r},t)$, eq. (7) holds for each particle $i = 1, ..., N$.

With respect to the simulations, the main idea is as follows: Instead of integrating the set of the coupled eqs. (1), (2), now the stochastic motion of the particles of component C_n is simulated. The advantage of this procedure results from the fact that in the Langevin eq. (7), the gradient $\vec{\nabla} m(\vec{r},t)$ appears only in a *linear* manner. Hence, for the time step the restriction results:

$$\Delta t < \left(\alpha \left| \frac{\partial m(\vec{r},t)}{\partial \vec{r}} \right| \right)^{-1} \tag{8}$$

which has to be compared to eq. (6). One could argue, that for an appropriate particle-based simulation of reaction-diffusion equations, a large number of coupled Langevin equations needs to be solved. This might be considered a disadvantage which compensates the advantage of a fast algorithm. But, as Schimansky-Geier *et al.* have shown [16, 17] already the consideration of about 10^4 particles results in sufficently smooth patterns.

As another advantage, the particle-based approach is also applicable in cases where only *small particle numbers* govern the structure formation, like in gas discharges [25], on catalytic surfaces [14], in cell membranes [7], or during cell migration [15]. Here, the continuous limit becomes questionable and partial differential equations are not sufficient to describe the behavior of the system. The final pattern is *path-dependent*, which means it is intrinsically determined by the history of its creation and irreversibility and early symmetry breaks play a considerable role (cf. also [20]). Hence, a stochastic description is needed which considers fluctuations in the system.

2 Active Brownian Particles

So far, we have introduced two different levels of description for the particles of component C_n: the "individual" description by means of Langevin eq. (7), and the density description by means of Fokker-Planck equation (2), (5) respectively. In the limit of a large number of particles, $N \to \infty$, both descriptions will of course lead to equivalent results.

The particles of component C_n are denoted as *active Brownian particles*. These are Brownian particles which motion can be described by a Langevin equation, but additionally, they are also *active* in the sense, that they are able to generate a self-consistent field, which in turn influences their further movement and physical or chemical behavior. This non-linear feedback between the particles and the field results in an interactive structure formation process on the macroscopic level. Hence, these models have been used to simulate a broad variety of pattern formation processes in complex systems, ranging from physical to biological and social systems [8, 17, 19–21].

The motion of "usual" Brownian particles would be rather considered as *passive motion*, simply because the Brownian particle does not play an active part in this motion. The motion of *active* Brownian particles, however, is strongly influenced by the gradients of the field created by themselves. A more refined description should therefore consider that the *activity* of the particles, i.e. the generation of a self-consistent field would require some *energy*. This holds especially if we want to describe phenomena such as the aggregation of biological species, as mentioned in the previous section. Here, the individuals of the species first need some energy in order to produce the chemical field used for their communication. That means the production term in eq. (3) should be substantiated by some energetic considerations.

In recent papers, the concept of active Brownian particles has been extended by considering that the active particles have the ability to take up energy from the environment, to store it in an internal energy depot [3,18] and to convert internal energy to perform different activities, such as metabolism, motion, change of the environment, or signal-response behavior. The resulting balance equation for the internal energy depot, e, of an active Brownian particle is then given by:

$$\frac{d}{dt}e(t) = q(\vec{r}) - s - c\, e(t) - d(\vec{v})\, e(t) \tag{9}$$

$q(\vec{r})$ shall be the space-dependent flux of energy into the depot. The internal energy will be decreased by three different processes: (i) generation of a self-consistent field $m(\vec{r},t)$ at a rate s, (ii) internal dissipation, which is assumed to be proportional to the depot energy, c being the rate of energy loss, (iii) acceleration of motion, i.e. conversion of internal into kinetic energy, where the rate $d(\vec{v})$ should be a function of the actual velocity of the particle. A simple ansatz for $d(\vec{v})$ reads $d(\vec{v}) = d_2 v^2$, with $d_2 > 0$.

Because of the acceleration of the Brownian particle in the direction of movement, the equation of motion has to consider an additional driving force, $d_2 e(t)\vec{v}$ [3,18]. Hence, the Langevin equation for particle i with mass $m = 1$ should read now:

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i \quad ; \quad \frac{d\vec{v}_i}{dt} = -\gamma_0 \vec{v}_i + d_2 e(t)\vec{v} + \alpha' \left.\frac{\partial m(\vec{r},t)}{\partial \vec{r}}\right|_{\vec{r}_i} + \sqrt{2\,S}\,\vec{\xi}_i(t). \tag{10}$$

Here, γ_0 is the friction coefficent of the moving particle, $\alpha' = \alpha\gamma_0$, and S is the strength of the stochastic force, which is related to the diffusion constant D_n via the fluctuation-dissipation theorem: $S = k_B T \gamma_0 = D_n \gamma_0^2$.

The equation of motion for the active Brownian particles, eq. (10), is coupled (i) to the equation for the energy depot $e(t)$, eq. (9), and (ii) to the equation of the self-consistent field $m(\vec{r},t)$, eqs. (1), (3). We may assume a constant influx of energy into the internal depot, $q(\vec{r}) = q_0$, and a fast relaxation of the internal energy depot, eq. (9), which reads in an adiabatic approximation:

$$e_0 = \frac{q_0 - s}{c + d_2 \vec{v}^2}. \tag{11}$$

The Langevin eq. (10) can then be written in the form:

$$\dot{\vec{v}}_i = -\gamma(\vec{v})\vec{v}_i + \alpha'\vec{\nabla}m(\vec{r},t) + \sqrt{2\,S}\,\vec{\xi}_i(t) \tag{12}$$

where $\gamma(\vec{v})$ now denotes a *velocity dependent nonlinear friction function*:

$$\gamma\,(\vec{v}) = \gamma_0 - \frac{(q_0 - s)\,d_2}{c + d_2\vec{v}^2}\ . \tag{13}$$

Dependent on the parameters γ_0, d_2, q_0, s, c, the friction function, eq. (13), may have a zero, where the friction is just compensated by the energy supply. It reads in the considered case:

$$\vec{v}_0^2 = \frac{q_0 - s}{\gamma_0} - \frac{c}{d_2} \tag{14}$$

We see that for $\vec{v} < \vec{v}_0$, 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.

Negative friction plays an important role e.g. in technical constructions or in the theory of sound developed by Rayleigh [13] already at the end of the last century. Here, the velocity-dependent friction function can be expressed as:

$$\gamma(\vec{v}) = -\gamma_1 + \gamma_2\,\vec{v}^2 = \gamma_1\left(\frac{\vec{v^2}}{\vec{v}_0^2} - 1\right) \tag{15}$$

This Rayleigh-type model is a standard model for self-sustained oscillations studied also in the context of Brownian motion [10]. We note that $\vec{v}_0^2 = \gamma_1/\gamma_2$ defines here the special value where the friction function, eq. (15), is zero (cf. Fig. 1). Another example for a velocity dependent friction function with a zero $\vec{v}_0$ introduced in [15], reads:

$$\gamma(\vec{v}) = \gamma_0\left(1 - \frac{\vec{v}_0}{\vec{v}}\right) \tag{16}$$

It has been shown that eq. (16) allows to describe the active motion of different cell types, such as granulocytes, monocytes or neural crest cells [15]. Here, the speed $\vec{v}_0$ expresses the fact that the motion of cells is not only driven by stochastic forces, instead cells are also capable of self-driven motion.

Compared to eqs. (15), (16), the velocity-dependent friction function in eq. (13) is bound to a maximum value γ_0 reached for $\vec{v} \to \infty$ and avoids the singularity for $\vec{v} \to 0$ on the other hand (cf. Fig. 1).

Provided a supercritical influx of energy, i.e. for $\vec{v}_0 > 0$, the passive motion of "usual" Brownian particles could be transformed into *active motion*. In this state, the energy can be used for the

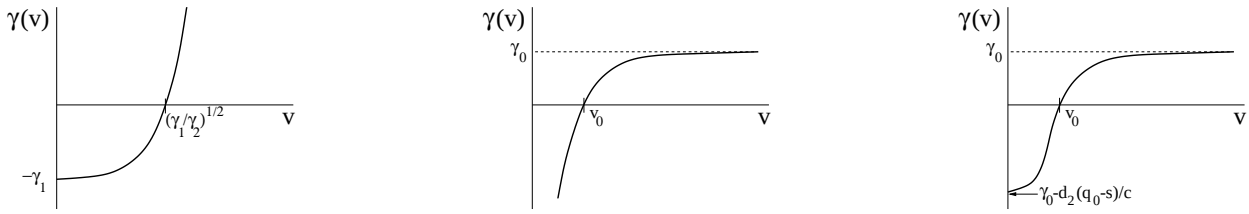

Figure 1: Different types of a velocity-dependent friction function, $\gamma(\vec{v})$ with a zero $\vec{v}_0$. (left) eq. (15), (middle) eq. (16), (right) eq. (13). For $\gamma(\vec{v}) < 0$ "pumping" dominates, while for $\gamma(\vec{v}) > 0$ "dissipation" dominates.

acceleration of the particles and the generation of the self-consistent field. Due to the pumping mechanism introduced in our model, the conservation of energy clearly does not hold for the active particles, i.e. we now have a non-equilibrium, canonical-dissipative system [6] (cf. also the paper of W. Ebeling in this book). The distribution function $P(\vec{r},\vec{v},t)$ which corresponds to the Langevin eq. (12) can be described by a Fokker-Planck equation of the form:

$$\begin{aligned}\frac{\partial P(\vec{r},\vec{v},t)}{\partial t} &= \frac{\partial}{\partial \vec{v}}\left\{\gamma(\vec{v})\,\vec{v}\,P(\vec{r},\vec{v},t) + S\,\frac{\partial P(\vec{r},\vec{v},t)}{\partial \vec{v}}\right\} \\ &\quad -\vec{v}\,\frac{\partial P(\vec{r},\vec{v},t)}{\partial \vec{r}} + \alpha'\nabla m(\vec{r})\,\frac{\partial P(\vec{r},\vec{v},t)}{\partial \vec{v}} \end{aligned} \tag{17}$$

In [5], we have investigated the solutions of eq. (17) for different special cases, which also include the nonlinear friction functions of eqs. (13)-(16). For a subcritical pumping of energy, we found an *unimodal velocity distribution*. This is the case of the *passive mode* of motion which corresponds to the *Maxwellian velocity distribution*. However, for supercritical pumping, a *crater-like velocity distribution* results. The corresponding *active mode* for the stationary motion is described by strong deviations from the Maxwell distribution. This active mode of motion will be further investigated in the following section.

3 Motion of Active Brownian Particles in External Potentials

Active motion is of interest for the dynamics of *driven systems*, such as physico-chemical [12] or biological [15] systems. However, recent models on self-driven particles often neglect the energetic aspects of active motion while focusing on the interaction of particles [1, 9, 24]. In our model, the interaction between the active particles is decribed by the self-consistent field, $m(\vec{r},t)$ generated by them. The coupling parameter s represents the amount of energy per time unit, which each particle spends on its interaction with other particles. Instead of a self-consistent field, the interaction between the particles may be also described by an interaction potential. e.g. a Toda potential [11].

Alternatively, we may also consider the interaction via global coupling, e.g. via invariants of the system, such as the total momentum or the total angular momentum [4].

For the further discussion, we will neglect the interaction of the particles via a self-consistent field, i.e. $s \to 0$. The spatio-temporal field $m(\vec{r},t)$, which is not created in this case, shall be replaced by a time-independent spatial potential $U(\vec{r})$, which may result in an external force on the particles. Assuming again that the internal energy depot of the active particles relaxes fast, the resulting Langevin equation reads now:

$$\dot{\vec{v}} = -\left(\gamma_0 - \frac{q_0\, d_2}{c + d_2\vec{v}^2}\right)\vec{v} + \vec{\nabla}U(\vec{r}) + \sqrt{2\,S}\,\vec{\xi}(t) \tag{18}$$

Let us first discuss the deterministic case. With $S = 0$ and $\vec{F} = -\vec{\nabla}U(\vec{r})$, the stationary solutions of eq. (18) result from the equation:

$$\left[d_2\gamma_0\, v_0^2 - d_2\vec{F}\vec{v}_0 - (q_0 d_2 - c\gamma_0)\right]\vec{v}_0 = c\vec{F}. \tag{19}$$

Depending on the value of $\vec{F}$ and in particular on the sign of the term $(q_0 d_2 - c\gamma_0)$, eq. (19) has either one or three real solutions for the stationary velocity, $\vec{v}_0$. The always existing solution expresses a direct response to the force in the form: $\vec{v}_0(\vec{r}) \sim \vec{F}(\vec{r})$. This solution results from the analytic continuation of Stokes' law, $\vec{v}_0 = \vec{F}/\gamma_0$, which is valid for $d_2 = 0$. We will denote this solution as the "normal response" mode of motion, since the velocity $\vec{v}$ has the same direction as the force $\vec{F}$ resulting from the external potential $U(\vec{r})$. 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, $\vec{v}_0$, 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*.

Figure 2: (right) Sketch of the one-dimensional motion of the particle in the presence of a constant force $\vec{F} = -\vec{\nabla}U(x)$ =const. (left) Stationary velocities $\vec{v}_0$, eq. (19), vs. conversion rate d_2. Parameters: $\vec{F} = +7/8$, $q_0 = 10$, $\gamma_0 = 20$, $c = 0.01$. [22]

In order to elucidate this, we consider the case of a one-dimensional linear potential $U(x) = -ax$ as shown in Fig. 2. The energy supply from the internal depot is described by the parameter d_2. Fig. 2 shows that with increasing d_2 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*, above a critical value of d_2, in the active mode a high-velocity motion *against* the direction of the force $\vec{F}$ becomes possible. This is indicated in Fig. 2 by a negative stationary velocity which corresponds to an "uphill" motion. We note that a stability analysis for the "uphill" motion and a detailed investigation of the critical energy supply has been carried out in [22], while in [22,23] applications to a piesewise linear periodic potential (ratchet potential) have been discussed. For instance, above a critical energy supply we observed the directed motion of an ensemble of active Brownian particles.

Let us eventually discuss the motion of active Brownian particles in a two-dimensional parabolic potential:

$$U(x_1, x_2) = \frac{1}{2} a \, (x_1^2 + x_2^2) \tag{20}$$

For a subcritical supply of energy, the particles position will fluctuate around the origin of the potential. For a supercritical supply, however, we find the motion of the particles on a stochastic limit cycle [3,5,18]. This is also shown in Fig. 3 for an ensemble of active particles which start with an empty internal energy depot. In this particular simulation, the initial position was the same for all particles and different from the potential minimum. Thus, for intermediate times, the motion of the particle ensemble reminds on *swarming*, i.e. a coherent motion with slow spatial dispersion. After an inital stage, we find the occurence of two branches of the swarm which results from a symmetry break (cf. Fig. 3 a). These two branches will, after a sufficient long time, move on two limit cycles (as already indicated in Fig. 3 b). One of these limit cycles refers to the left-handed, the other one to the right-handed direction of motion in the 2d-space.

Figure 3: Snapshots of a swarm of $N = 2000$ active Brownian particles moving in a two-dimensional potential, eq. (20). (left) $t = 15$, (right) $t = 99$. Initial conditions for all particles: $x_1 = 0.0$, $x_2 = 0.5$, $v_1 = 0.0$, $v_2 = 0.0$, $e(0) = 0$. Parameters: $q_0 = 10$; $c = 1.0$; $\gamma_0 = 20$, $d_2 = 10$. [4]

The radius of the limit cycles obeys the relation [5]:

$$r_0^2 = \frac{v_0^2}{a} \tag{21}$$

where v_0 is the stationary velocity of the particles on the limit cycle. It has been shown [3] that for the case of a parabolic potential, v_0 has the same value as for the force-free case ($U = 0$), namely:

$$\vec{v}_0^2 = \frac{q_0}{\gamma_0} - \frac{c}{d_2} \tag{22}$$

The total mechanical energy of an active particle moving on the limit cycle can then be expressed as:

$$E_0 = \frac{1}{2}(v_1^2 + v_2^2) + \frac{a}{2}(x_1^2 + x_2^2) = \frac{1}{2}v_0^2 + \frac{a}{2}r_0^2 \tag{23}$$

In [3] we have shown that any initial value of the energy converges (at least in the limit of strong pumping) to

$$H \longrightarrow E_0 = v_0^2 \tag{24}$$

This corresponds to an equal distribution between kinetic and potential energy, i.e. similar to the harmonic oscillator in one dimension, both parts contribute the same amount to the total energy. We note that the theoretical results of eqs. (21)-(24) agree perfectly with the results of computer simulations of N active particles which move according to the Langevin eq. (10), coupled with eq. (9) for the internal energy depot.

Acknowledgement

The author is very indebted to LSG for a long-lasting and stimulating collaboration. Further, I would like to thank W. Ebeling (Berlin) and B. Tilch (Stuttgart) for collaboration.

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