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Complex Motion of Brownian Particles with Energy Supply

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Abstract

We study a model of Brownian particles which are pumped with energy by means of a non-linear friction function. Analytical solutions of the corresponding Fokker-Planck equation are presented and compared with computer simulations. Different to the case of passive Brownian motion, we find several new features of the dynamics, such as the formation of limit cycles, a large mean squared displacement which increases quadratically with the energy supply, or non-equilibrium velocity distributions with crater-like form. In the four-dimensional phase space, the corresponding distribution has the form of two hoops or two tires. Further, the general features of motion in arbitrary two-dimensional potentials are discussed within a diffusion approximation.

Introduction

Active motion, which relies on the supply of energy from the surroundings, is of interest for the dynamics of *driven systems*, such as physico-chemical [1, 2], biological [3] or even traffic systems [4]. However, recent models on self-driven particles often neglect the energetic aspects of active motion while focusing on the interaction of particles [4–6]. On the other hand, there exist different approaches dealing with the distribution of energy in non-linear systems [7, 8].

In order to describe active motion in the presence of stochastic forces, we have suggested a model of *active Brownian particles*, which have the ability to take up energy from the environment, to store it in an internal energy depot and to convert internal into kinetic energy [9–13]. Provided a supercritical supply of energy, these particles can move in an "high-velocity" or active mode, which results in different types of complex motion.

The main objective of this work is to study the influence of noise on active particles and the corresponding probability distributions. First, we investigate the force-free motion of pumped Brownian particles, which may be described by a non-Maxwellian velocity distribution. Then, the results are generalized for different types of two-dimensional external potentials.

Motion of Free Particles

The motion of a Brownian particle with mass m, position $\boldsymbol{r}$, and velocity $\boldsymbol{v}$ moving in a space-dependent potential, $U(\boldsymbol{r})$, can be described by the following Langevin equation:

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

Here, $\gamma(\boldsymbol{v})$ is the coefficient of active friction, which is assumed to depend on velocity. Several aspects of an additional *space* dependence were discussed in an earlier work [14]. $\mathcal{F}(t)$ is a stochastic force with strength D and a δ-correlated time dependence. In the case of thermal equilibrium systems, with $\gamma(\boldsymbol{v}) = \gamma_0 = \text{const.}$, we may assume that the loss of energy resulting from friction, and the gain of energy resulting from the stochastic force, are compensated in the average. Then the fluctuation-dissipation theorem (Einstein relation) applies: $D = \gamma_0\, k_B T/m$, where T is the temperature and k_B is the Boltzmann constant.

In this paper we are mainly interested in stochastic effects and in particular in the probability density $P(\boldsymbol{r}, \boldsymbol{v}, t)$ to find the particle at location $\boldsymbol{r}$ with velocity $\boldsymbol{v}$ at time t. As well known, the distribution function $P(\boldsymbol{r}, \boldsymbol{v}, t)$ which corresponds to the Langevin Eq. (1), can be described by a Fokker-Planck equation (FPE). In the special case $\gamma(\boldsymbol{v}) = \gamma_0$ the stationary solution of this FPE, $P^0(\boldsymbol{r}, \boldsymbol{v})$, is given by the Boltzmann distribution. However, if we consider an energy supply by means of a velocity dependent friction function, $\gamma(\boldsymbol{v})$, this will result in significant differences to the stationary distribution, as shown below. We will use here the following ansatz [9, 10]:

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

which is plotted in Fig. 1. We see that 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. The friction function, Eq. (2), has a zero for:

$$\boldsymbol{v}_0^2 = \frac{q_0}{\gamma_0} - \frac{c}{d_2} \tag{3}$$

We restrict the further discussion to the two-dimensional space $\boldsymbol{r} = \{x_1, x_2\}$. Then the stationary velocities v_0, Eq. (3), where the friction is just compensated by the energy supply, define a cylinder in the four-dimensional space, $v_1^2 + v_2^2 = \boldsymbol{v}_0^2$, which attracts all deterministic trajectories of the dynamic system. The stationary solution of the FPE reads for the friction function, Eq. (2), and in the absence of an external potential, i.e. $U(x_1, x_2) \equiv 0$:

$$P^0(\boldsymbol{v}) = C' \left(1 + \frac{d_2 \boldsymbol{v}^2}{c}\right)^{\frac{q_0}{2D}} \exp\left(-\frac{\gamma_0}{2D}\, v^2\right) \tag{4}$$

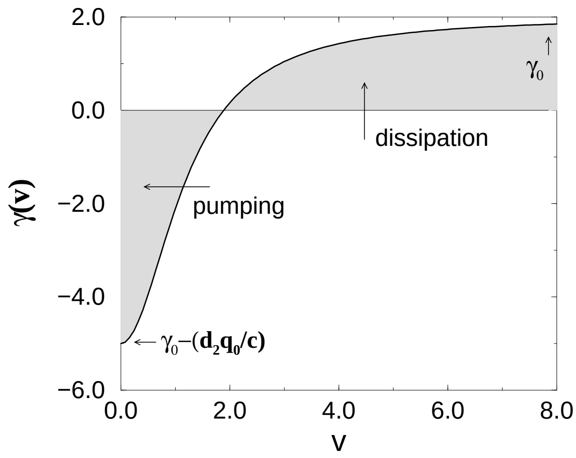

Figure 1: Velocity-dependent friction function $\gamma(v)$, Eq. (2) vs. velocity v. The velocity ranges for "pumping" ($\gamma(v) < 0$) and "dissipation" ($\gamma(v) > 0$) are indicated. Parameters: $q_0 = 10$; $c = 1.0$; $\gamma_0 = 2$, $d_2 = 0.7$.

Compared the Maxwellian velocity distribution of "simple" Brownian particles, a new pre-factor appears now in Eq. (4) which results from the internal energy depot. For a subcritical pumping of energy, $q_0 d_2 < c\gamma_0$, an *unimodal velocity distribution* results, centered around the maximum $\boldsymbol{v}_0 = 0$. This is the case of the "low velocity" or *passive mode* for the stationary motion which here corresponds to the *Maxwellian velocity distribution.* However, for supercritical pumping, $q_0 d_2 > c\gamma_0$, a *crater-like velocity distribution* results which is also shown in Fig. 2. The maxima of $P^0(\boldsymbol{v})$ correspond to the solutions for $\boldsymbol{v}_0^2$, Eq. (3). The corresponding "high velocity" or *active mode* for the stationary motion is described by strong deviations from the Maxwell distribution.

In the limit of strong noise $D \sim T \to \infty$, i.e. at high temperatures, we get from Eq. (4) the known Maxwell distribution by means of the Einstein relation. In the other limiting case of strong activation, i.e. relatively weak noise $D \sim T \to 0$ and/or strong pumping, we find a δ-distribution instead:

$$P_0(\boldsymbol{v}) = C\delta\left(\boldsymbol{v}^2 - \boldsymbol{v}_0^2\right) \; ; \quad \left\langle \boldsymbol{v}^2 \right\rangle = \boldsymbol{v}_0^2 \tag{5}$$

Treating this limiting case as suggested in [2, 3], we introduce an amplitude-phase representation in the velocity-space. After a separation of the variables, we find that the distribution of angels satisfies a diffusion equation, with $D_\varphi = D/v_0^2$ being the angular diffusion constant. By means of

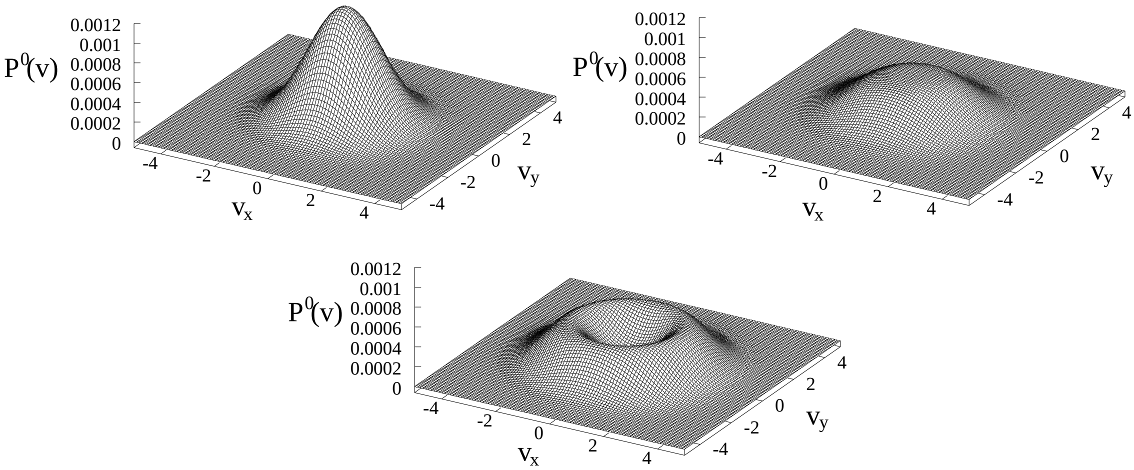

Figure 2: Normalized stationary solution $P^0(\boldsymbol{v})$, Eq. (4), for $d_2 = 0.07$ (top left), $d_2 = 0.2$ (top right) and $d_2 = 0.7$ (bottom). Other parameters: $\gamma_0 = 2$, $D = 2$, $c = 1$, $q_0 = 10$. Note that $d_2 = 0.2$ is the bifurcation point for the given set of parameters.

this, we find after some calculations the effective spatial diffusion constant as:

$$D_r^{\text{eff}} = \frac{2v_0^4}{D} = \frac{2}{D}\left(\frac{q_0}{\gamma_0} - \frac{c}{d_2}\right)^2 \tag{6}$$

Due to the additional pumping by means of the friction function, $\gamma(\boldsymbol{v})$, we obtain a high sensitivity with respect to noise expressed in the scaling with $(1/D)$.

Motion in External Potentials

In the following, we discuss the motion in a two-dimensional external potential, $U(x_1, x_2)$, which results in additional forces on the pumped Brownian particle. The case of a constant external force was experimentally and theoretically investigated in [3]. We consider here a parabolic potential [13]

$$U(x_1, x_2) = \frac{1}{2} a\,(x_1^2 + x_2^2) \tag{7}$$

The *deterministic* motion of the pumped Brownian particle is now described by four coupled first-order differential equations [13]. The trajectory defined by these four equations is like a hoop in the four-dimensional space. Most projections to the two-dimensional subspaces are circles or ellipses; however there are two subspaces, namely $\{x_1, v_2\}$ and $\{x_2, v_1\}$, where the projection is like a rod [13]. A second limit cycle is obtained by time reversal, $t \to -t$, $v_1 \to -v_1$, $v_2 \to -v_2$. This limit cycle also forms a hula hoop which is different from the first one in that the projection to the

$\{x_1, x_2\}$ plane has the opposite rotation direction compared to the first one. However both limit cycles have the same projections to the $\{x_1, x_2\}$ and to the $\{v_1, v_2\}$ plane. The separatrix between the two attractor regions is given by the plane $(v_1 + v_2 = 0)$ in the four-dimensional space.

In the *stochastic* case, we find that the two hoop rings are converted into a distribution looking like two embracing hoops with finite size, which for strong noise convert into two embracing tires in the four-dimensional space, as shown in Fig. 3. While in the deterministic case either left- or righthanded rotations are found, in the stochastic case the system may switch randomly between the left- and righthand rotations, since the separatrix becomes transparent.

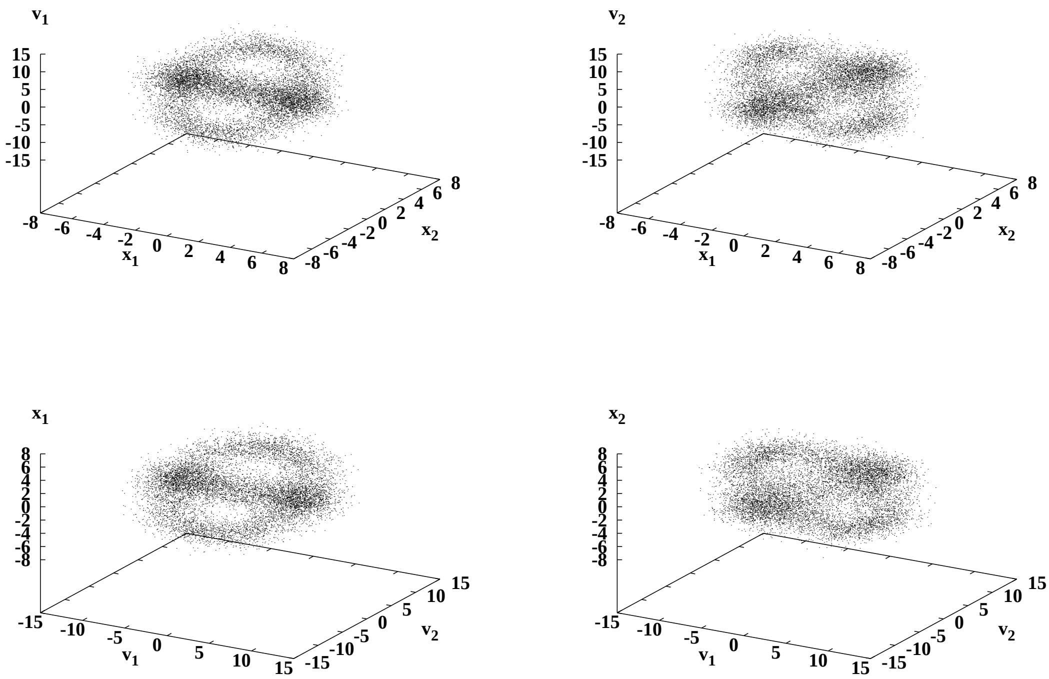

Figure 3: Projections of a stochastic trajectory on the three-dimensional subspaces $\{x_1, x_2, v_1\}$, $\{x_1, x_2, v_2\}$, $\{v_1, v_2, x_1\}$ and $\{v_1, v_2, x_2\}$. The trajectory was obtained with long time computer simulations of Eq. (1) with constant energy supply at a noise strength of $D = 0.8$. Other parameters are: $\gamma_0 = 0.2$, $c = 0.01$, $d_2 = 0.1$, $a = 2.0$ and $q_0 = 10.0$.

In order to get the explicite form of the distribution in the stochastic case we may introduce the amplitude-phase representation

$$
\begin{aligned}
x_1 &= \varrho\,\cos(\omega t+\varphi) \qquad & v_1 &= \; -\varrho\,\omega\,\sin(\omega t+\varphi)\\
x_2 &= \varrho\,\sin(\omega t+\varphi) \qquad & v_2 &= \;\varrho\,\omega\,\cos(\omega t+\varphi)
\end{aligned}
\tag{8}
$$

where the radius ϱ is now a slow *stochastic variable* and the phase φ is a fast *stochastic variable*. By using the standard procedure of averaging with respect to the fast phases we get the following stationary solution for the distribution of the radii:

$$
P^0(\varrho) \simeq \left(1+\frac{d_2}{c}a\varrho^2\right)^{\frac{q_0}{2D}} \exp\left(-\frac{\gamma_0}{D}a\varrho^2\right)
\tag{9}
$$

We find that the maximum is located at

$$
\varrho^2 = r_0^2 = \omega^2 v_0^2 = \left(\frac{q_0}{\gamma_0}-\frac{c}{d_2}\right)\omega^2
\tag{10}
$$

For the harmonic potential the equal distribution between potential and kinetic energy, $mv_0^2 = ar_0^2$, is valid, which leads to the relation: $\omega_0 = v_0/r_0 = \omega$. For other potentials $U(r)$, this relation has to be replaced by the condition that on the limit cycle the attracting radial forces are in equilibrium with the centrifugal forces. This condition leads to $v_0^2/r_0 = |U'(r_0)|$. For a given v_0, it defines an implicit relation for the equilibrium radius: $v_0^2 = r_0\,|U'(r_0)|$. Then the frequency of the limit cycle oscillations is given by:

$$
\omega_0^2 = \frac{v_0^2}{r_0^2} = \frac{|U'(r_0)|}{r_0}
\tag{11}
$$

In the case of linear oscillators this leads to $\omega_0 = a^{1/2}$ as before.

Diffusion Approximation

We consider now the transition to the so-called overdamped approximation. As well known, for the limit case of strong damping (γ_0 large) and no pumping ($\gamma\left(\boldsymbol{v}^2\right) = \gamma_0 = \text{const.}$) the Fokker-Planck equation can be reduced to a Smoluchowski equation. A similar reduction is also possible for the limit of strong activation. For free particles we may use the results obtained above. According to Eq. (6), the *spatial* distribution function satisfies the diffusion equation:

$$
\frac{\partial}{\partial t}P\left(x_1,x_2,t\right) = D_r^{\text{eff}}\,\Delta P\left(x_1,x_2,t\right)
\tag{12}
$$

In order to get explicite solutions for the full problem we have to solve the equations for the subspaces for φ and r, where we have free diffusion. The complete solution for free particles with arbitrary initial conditions reads:

$$P\left(x_1 x_2 v_1 v_2 t\right) = C\,\delta\left(v_1^2+v_2^2-v_0^2\right)\int_0^{2\pi} d\varphi' P\left(\varphi',0\right)\exp\left(-\frac{(\varphi-\varphi')^2}{D_\varphi t}\right) \times \int dx_1'\,dx_2'\,P\left(x_1 x_2 t\right)\exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}')^2}{4D_r^{\mathrm{eff}}\,t}\right) \tag{13}$$

We note that due to D_r^{eff}, Eq. (6), the mean squared displacement $\left\langle(\Delta r)^2\right\rangle_t$ resulting from Eq. (13) increases quadratically with the supercritical energy supply, and scales as $(1/D)$.

For the particles motion in a potential U we postulate the following generalization:

$$\frac{\partial}{\partial t}P\left(x_1 x_2 t\right) = D_r^{\mathrm{eff}}\nabla\left\{\nabla P\left(x_1 x_2\right) + \frac{1}{D_v}\gamma\left(\varrho_U\left|\nabla U\right|\right)\nabla U\left(x_1 x_2\right)P\left(x_1 x_2\right)\right\} \tag{14}$$

where $\gamma(\boldsymbol{v}^2)$ is the friction function defined by Eq. (2). A strict derivation of Eq. (14) is not yet available, we note however the following properties:

(i) In the force-free case Eq. (12) is obtained.

(ii) The maximum of the stationary solution corresponds to the local equilibrium curves defined by $\gamma\left(\varrho_U\left(x_1 x_2\right)\left|\nabla U\left(x_1 x_2\right)\right|\right)=0$ which guarantees the equilibrium of the centrifugal forces.

(iii) For the harmonic oscillator the explicite stationary solution of Eq. (14) is compatible with the solution of the Fokker-Planck equations.

For the special case of a parabolic potential, the dynamics of the particles includes rotations, as shown above. Therefore, the probability flux, which can be derived from Eq. (14) will contain additional contributions corresponding to left/right rotational flows. The possible directions are equally probable, i.e. in long time average the rotational flow is zero. However, the transition times between the two modes may be very long.

Discussion

In this paper we have investigated the influence of noise on active Brownian particles, which are driven by energy obtained from a non-linear friction function. As we have shown, in this case new dynamical features occur, such as:

(i) new diffusive properties with large mean square displacement,

(ii) non-equilibrium velocity distributions with crater-like shape,

(iii) the formation of limit cycles corresponding to left/righthand rotations.

Qualitative similar features are obtained for the motion of driven particles in physico-chemical systems, for example for the motion of liquid droplets on hot surfaces, or the motion of surface-active solid particles [2]. There are also relations to active biological motion [3]. In this paper, we did not intend to model any particular object but analyzed the general physical non-equilibrium properties of such systems. While our investigations are based on rather simple physical assumptions on non-linear friction for Brownian particles, we found a rich dynamics, which might be of interest for more applied investigations later.

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