DIFFUSION OF ACTIVE BROWNIAN PARTICLES

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1. Introduction

Active motion is one of the most fascinating aspects of biological systems. This motion can appear in many different biological contexts either inside cells or on the multi-cellular level. Moreover, active motion may appear as a collective property of many organisms, as for example in the movement of whole flocks of animals [1].

Simple phenomenological models may help us to understand the dynamics of active entities, their statistical properties, and possibly how their dynamics and statistics are related to the biological task (for instance, transport of proteins for molecular motors or food search for the motion of animals). One class of models studied during the last 20 years are active Brownian particles. These models not only take into account random influences on the biological object from its surrounding, dissipation of the object´s energy, but also uptake of energy (negative dissipation). The latter is often realized by a friction coefficient which depends nonlinearly on particle´s speed and attains negative values for low speed.

According to the classical theory the motion of a Brownian particle (BP) with the mass m and radius R in a fluid is described by the Langevin equation (LE)

$$m\dot{\upsilon} = -\gamma\upsilon + \sqrt{2D}\,\xi\left(t\right), \tag{1}$$

where $x(t)$ and $\upsilon(t) = \dot{x}$ are the particle position and velocity, respectively. The resistance force against the particle motion is the Stokes friction force proportional to the velocity, and the irregular impulses from the surrounding molecules are described by the (white) noise force ~ $\xi(t)$ with the properties $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \delta(t - t')$. In Eq.(1), $D = k_B T\gamma$ is the noise intensity (k_B is the Boltzmann constant, T is the temperature and $\gamma = 6\pi R\eta$ is the friction coefficient proportional to the dynamic viscosity η of the surrounding fluid). The diffusion coefficient of the particle, which also determines the intensity of the noise generated by Eq.(1), is given by the Einstein formula $D_0 = \gamma^{-2}D$.

In this paper we study a generalization of this theory to the case when the friction coefficient γ and the noise intensity are functions of velocity. We derive a general formula for the diffusion coefficient of BPs in equilibrium systems. This formula is then applied to three different friction functions, taken from current models of active Brownian motion. First, we replace γ with the friction function [2]

$$\gamma(\upsilon) = \gamma\upsilon^{2\alpha}, \tag{2}$$

where α is a constant. Equation (1) can then be regarded as a generator of noise with very different properties from the white noise $\xi(t)$. In such a generator, the diffusion coefficient D_{eff} corresponds to the noise intensity of the velocity υ. It is of particular interest to know the properties of this quantity and its dependence on the system parameters D, γ, and m [2]. Our second example is a nonlinearly increasing friction function discussed in Ref. [3],

$$\gamma(\upsilon) = \gamma(1+\beta\upsilon^2), \tag{3}$$

where $\beta > 0$. This function can also be regarded as a Taylor expansion of a sufficiently smooth and symmetric friction function. Finally, in the simplified depot model proposed in [4] (the so-called SET model), the friction attains the form

$$\gamma(\upsilon) = \gamma\left[1 - \frac{\varepsilon}{1+\upsilon^2}\right], \quad \varepsilon < 1. \tag{4}$$

This nonlinear friction gives rise to self-propelled motion if $\varepsilon > 1$ when $\gamma(\upsilon)$ has zeros at $\upsilon = \pm\sqrt{\varepsilon - 1}$ and is negative at speeds between and positive beyond these values.

In the present contribution we consider equilibrium systems for which the fluctuation-dissipation theorem must hold. Then the LE for the motion of BP should contain a stochastic (or "spurious") force proportional to $\partial_\upsilon D(\upsilon)$ [3]. As distinct from Ref. [2] where this force was not included in the LE, here we take it into account.

2. The diffusion coefficient for active Brownian motion

The diffusion coefficient (we keep for it the same notation D_{eff} as in Ref. [2]) can be calculated from the mean square displacement of the particle as

$$D_{\text{eff}} = \lim_{t\to\infty} \frac{1}{2t}\left[x(t) - x(0)\right]^2, \tag{5}$$

or, using the Green-Kubo relation, $D_{\text{eff}} = \int_0^\infty \mathrm{d}\tau \left\langle \upsilon(t)\upsilon(t+\tau)\right\rangle$. Lindner´s theory [2] for the nonlinear BM incorporates the same random force as for the linear case. In the correct approach, when the friction force nonlinearly depends on the velocity υ, the random force for equilibrium systems should be changed: the intensity of the noise must also be the function of υ, as an implication of the fluctuation-dissipation theorem. Due to this fact we have to add a "stochastic" or the so called spurious force, proportional to the derivative of $D(\upsilon)$ [3] in the LE. Equation (1) then becomes

$$m\dot{\upsilon} = -\gamma(\upsilon)\upsilon - am^{-1}\partial_\upsilon D(\upsilon) + \sqrt{2D(\upsilon)}\xi(t), \tag{6}$$

where the properties of random function $\xi(t)$ are defined as before. Equivalent to the LE (6) is the Fokker-Planck equation for the distribution function $P(\upsilon, t)$ [5]

$$\partial_t P = m^{-2}\partial_\upsilon\left[D(\upsilon)\partial_\upsilon P\right] + m^{-1}\partial_\upsilon\left\{\left[\gamma(\upsilon)\upsilon + m^{-1}(a+1/2)\partial_\upsilon D(\upsilon)\right]\ P\right\}. \tag{7}$$

The equilibrium solution of Eq.(7) must have the form of the Maxwell-Boltzmann distribution. After substituting it into Eq.(7), the following fluctuation-dissipation relation for the case in question,

$$D(\upsilon) = k_B T\left[\gamma(\upsilon) + m^{-1}(a+1/2)\upsilon^{-1}\partial_\upsilon D(\upsilon)\right], \tag{8}$$

must reduce to the generalized Einstein relation $D(\upsilon) = k_B T\gamma(\upsilon)$, and hence the coefficient a in the equations of Langevin and Fokker-Planck must be $a = -1/2$.

Equation (8) can be established in different ways. Its most typical forms are: Ito´s [6], Stratonovich´s [7], and the kinetic´s form [3, 8], corresponding to a = 1/2, 0, and -1/2, respectively, and it is only in the last case that (8) coincides with the generalized Einstein relation [3].

In the kinetic interpretation, the FPE has the stationary solution $P_{st}(\upsilon) = (m/2\pi k_B T)^{1/2} \exp(-m\upsilon^2/2k_B T)$ and the exact formula for the effective diffusion coefficient D_{eff} for the natural boundary conditions $(\upsilon_{min} = -\infty,\ \upsilon_{max} = \infty)$ is given by the simple formula

$$D_{\mathrm{eff}} = \sqrt{\frac{m k_B T}{2\pi}} \int_{\upsilon_{\min}}^{\upsilon_{\max}} \gamma^{-1}(\upsilon) \exp\left[-U(\upsilon)\right] d\upsilon\,, \tag{9}$$

where $U(\upsilon) = m\upsilon^2/2k_B T$. We have derived this equation using the formula $D_{eff} = \langle \upsilon^2 \rangle \tau_{corr}$ [2] and Eq. S9.14 from Ref. [5] for the correlation time τ_{corr} of the function $\langle \upsilon(t)\upsilon(0)\rangle$.

Using Eq.(9), the diffusion coefficient for the friction function (2) reads

$$D_{\mathrm{eff}} = \frac{(k_B T)^{1-\alpha} m^{\alpha}}{2^{\alpha}\sqrt{\pi}\gamma} \Gamma\left(\frac{1}{2} - \alpha\right), \quad 2\alpha < 1. \tag{10}$$

This result coincides with the dimensional analysis. For all $\alpha < 1/2$ the diffusion coefficient is inversely proportional to the friction factor γ. For $\alpha \geq 1/2$, D_{eff} diverges. Note that D_{eff} increases with the increase of the particle mass m if $\alpha > 0$. For $\alpha = -1$ one has from (10) the simple relation $D_{eff} = (k_B T)^2/m\gamma$ and for constant γ we return to the Einstein theory.

As the next example, we consider the friction function (3). The analytical result for this friction is given by

$$D_{\mathrm{eff}} = \frac{1}{\gamma}\sqrt{\frac{\pi m k_B T}{2\beta}} \exp\left(\frac{m}{2k_B T\beta}\right) \mathrm{erfc}\left(\sqrt{\frac{m}{2k_B T\beta}}\right), \tag{11}$$

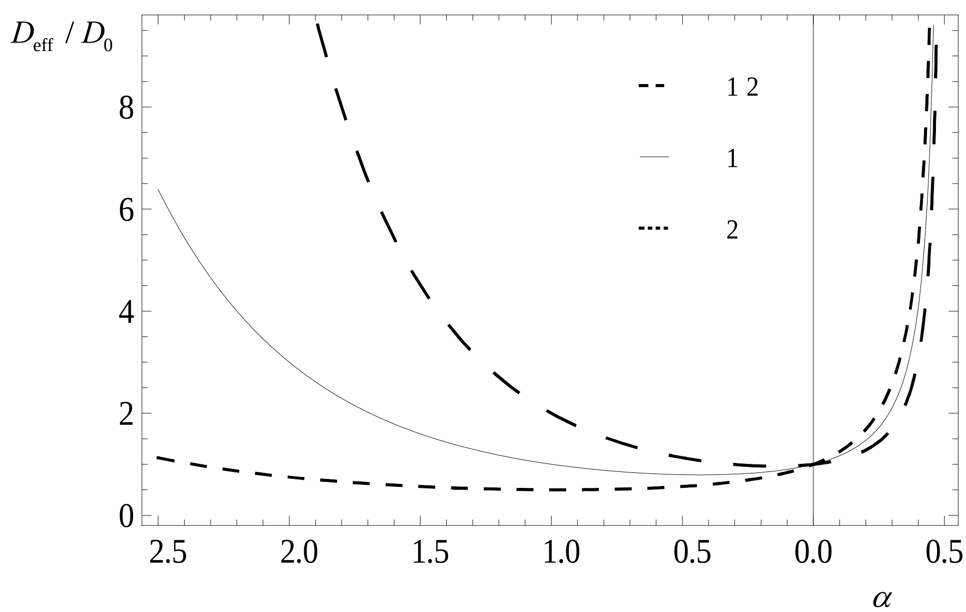
where erfc() is the complementary error function.

Finally, for the SET friction (4) the diffusion coefficient from Eq.(9) has the form

$$D_{\mathrm{eff}} = \frac{k_B T}{\gamma}\left[1 + \sqrt{\frac{\pi}{2}} \frac{\varepsilon}{\sqrt{1-\varepsilon}} \exp\left(\frac{1-\varepsilon}{2}\right) \mathrm{erfc}\left(\sqrt{\frac{1-\varepsilon}{2}}\right)\right]. \tag{12}$$

For such a system the diffusion coefficient does not depend on the mass m at all. In all the three cases, for normal BM ($\alpha = \beta = \varepsilon = 0$) the Einstein formula $D_{eff} = k_B T/\gamma$ is recovered.

In Fig.1, we show the diffusion coefficient as a function of α, $\langle \upsilon^2 \rangle\beta$, and ε, respectively, where $\langle \upsilon^2 \rangle = k_B T/m$ (equipartition theorem).



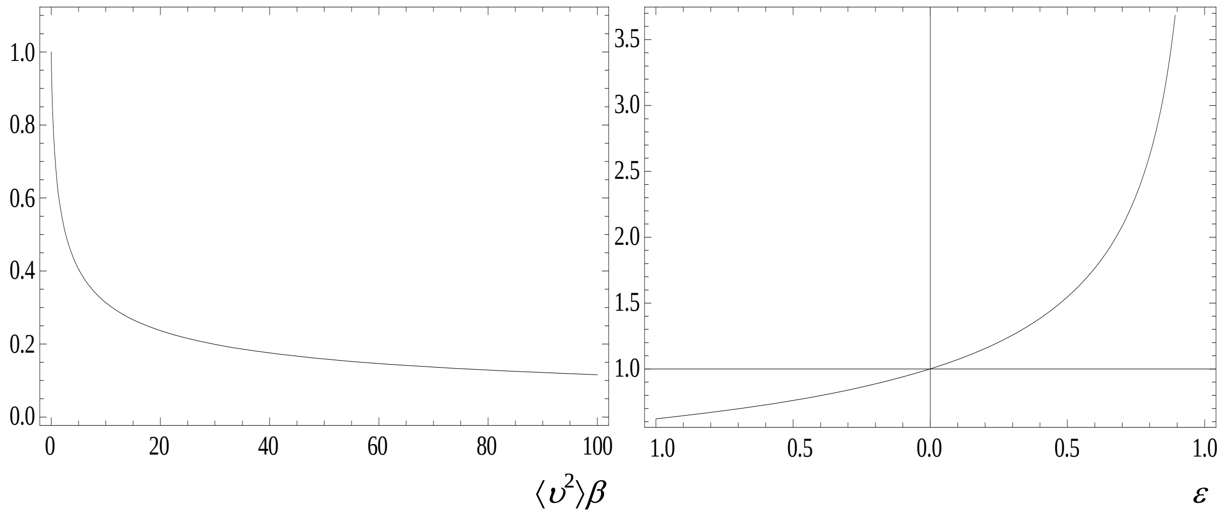


Fig.1: *Diffusion coefficient for friction laws (2), (3) and (4), respectively, normalized to the Einstein limit* $D_0 = k_B T/\gamma$. *The parameter* $\omega = \upsilon_c^2 / \langle \upsilon^2 \rangle$, *where* $\upsilon_c = (\gamma_0/\gamma)^{1/2\alpha}$.

3. Conclusion

In conclusion, we have studied the Brownian motion of particles in situations when the friction force nonlinearly depends on the particle velocity. The correspponding stochastic equations of motion are hardly solvable analytically. However, for stationary processes it was possible to obtain an exact expression for the particle diffusion coefficient, which also determines the intensity of the noise generated by the Langevin equation. For particles in equilibrium with their surrounding we used the kinetic conception of stochastic integration. The derived general formula for the diffusion coefficient has been applied to different frictions. Our choices were inspired by some actual models of active Brownian motors [2-5]. The main attention was given to the friction force proportional to $\upsilon^{2\alpha}\upsilon$. So far such force was studied using the strong assumption that the random force driving the particles is delta correlated in the time and its intensity is constant. Our results for equilibrium systems, for which the intensity of the random force should depend on the velocity, are very different. We have found the diffusion coefficient D_{eff} analytically and showed that it is finite only for $\alpha < 1/2$. For $\alpha = 0$ the obtained D_{eff} is the same as in the standard Einstein-Langevin theory. For all relevant α it is inversely proportional to the friction coefficient γ, but when $\alpha \neq 0$, D_{eff} in a non-trivial way scales with the particle mass and the temperature.

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