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The diffusion coefficient of nonlinear Brownian motion

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Abstract. Nonlinear Brownian motion (BM) refers to cases where the damping constant and possibly also the noise intensity in the Langevin equation depend on the velocity of the particle. Such velocity dependence is encountered in cases where Stokes' linear friction law does not apply, for relativistic Brownian particles, and for models of active motion of biological objects. For an arbitrary velocity dependence of damping and noise intensity, the diffusion coefficient can be given in terms of quadratures. We evaluate and discuss this quadrature formula for the three different cases. For a nonlinear friction (being larger at high speed than expected from Stokes' friction) and for the relativistic BM we obtain in general diffusion coefficients that are smaller than those for linear BM. The diminished diffusion in these equilibrium systems has different physical reasons. For the nonequilibrium model of active motion we demonstrate that diffusion can be minimized at a finite noise intensity.

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1. Introduction

Starting with the seminal work of Einstein [1], Brownian motion (BM) has been the subject of intense research over the past 100 years (see [2] and references therein). While the concept has been generalized in various directions (including anomalous diffusion, generalized Langevin equations, and others), the important issue of *nonlinear* BM has received comparably little attention.

Nonlinear BM refers to situations where an explicit velocity dependence of friction and diffusion coefficients has to be taken into account. This happens in at least three cases: if deviations from Stokes' law for the frictional force become important [3, 4], for relativistic BM [5], and for active BM describing self-propelled animal mobility [6]. The corresponding problem at the level of the Fokker–Planck equation is also encountered for a Wigner function in an optical lattice [7] and is related to the problem of anomalous diffusion.

Basic questions for these interesting equilibrium and nonequilibrium systems have not yet been answered. If dissipation and fluctuations increase at high speed stronger than expected for the classical BM will the spatial diffusion coefficient increase or decrease? What if we just assume Stokes' friction but consider a relativistic particle—does its diffusion coefficient exceed linear diffusion? Finally, for nonequilibrium models in which friction can be turned into a pumping term: how does diffusion depend on parameters in the model, in particular, on the strength of fluctuations?

In this paper we study a one-dimensional model of nonlinear BM

$$\dot{x} = v, \quad m\dot{v} = -\gamma(v)v + g(v)\xi(t), \tag{1}$$

where the general friction and noise functions $\gamma(v)$ and $g(v)$ are assumed to be symmetric in v and 'well-behaved' avoiding unphysical divergence of the velocity; in particular, the velocity can vary between two symmetric limiting values $\pm v_{\mathrm{M}}$. The noise $\xi(t)$ is Gaussian with $\langle\xi(t)\xi(t+\tau)\rangle = 2\delta(\tau)$. As for linear BM (where $\gamma(v) \equiv \gamma_0$ and $g(v) \equiv \sqrt{\gamma_0 k_{\mathrm{B}} T}$), the physical dimension of the friction function and noise prefactor are kg s^{-1} and kg m s$^{-3/2}$, respectively.

Equivalent to the Langevin equations (1) is the Fokker–Planck equation in velocity space

$$\partial_t P(v, t|v_0, 0) = \partial_v[\mu(v) + \partial_v g^2(v)/m^2]P(v, t|v_0, 0), \tag{2}$$

provided that we have decided upon an *interpretation* of the stochastic differential equation with multiplicative noise. The drift $\mu(v) = v\gamma(v)/m - qg(v)g'(v)/m^2$ will depend on the interpretation: those according to Ito [8, 9], Stratonovich [10, 11], and the so-called kinetic interpretation [3, 4, 12, 13] correspond to $q = 0, 1, 2$, respectively.

The central quantity of interest for BM is its effective diffusion coefficient

$$D_{\mathrm{eff}} = \lim_{t\to\infty} \langle(x(t) - x(0))^2\rangle/(2t).$$

Whereas in the classic linear case (with constant friction and noise functions $\gamma(v) \equiv \gamma_0$ and $g(v) \equiv \sqrt{\gamma_0 k_{\mathrm{B}} T}$, respectively), the diffusion coefficient is simply given by $k_{\mathrm{B}}T/\gamma_0$, for the nonlinear model (1) its calculation is nontrivial and may reveal interesting physics of equilibrium or nonequilibrium systems. The diffusion coefficient may even diverge (superdiffusion) for special functions $\gamma(v)$, $g(v)$. In this paper, however, the main concern is normal diffusion. For the diffusion coefficient a quadrature formula for the general one-dimensional case (1) is given and then evaluated and discussed for the different physical situations mentioned above.

2. Theory

The change in position can be expressed by $x(t) - x(0) = \int_0^t \mathrm{d}s\ v(s)$ according to (1). Assuming that the velocity correlation function decays sufficiently rapidly (i.e. has a finite correlation time), one arrives at the Kubo formula

$$D_{\mathrm{eff}} = \lim_{T\to\infty} \int_0^T \mathrm{d}s\ \langle v(0)v(s)\rangle_{\mathrm{st}} = \langle v^2\rangle \tau_{\mathrm{corr}}, \tag{3}$$

where the index 'st' indicates the autocorrelation function in steady state. By the last equality we expressed the diffusion coefficient by the correlation time of the velocity defined as the integral over the normalized autocorrelation function $\langle v(t)v(t+\tau)\rangle/\langle v^2\rangle$. Although an analytical expression for the correlation function in not feasible in general, the *correlation time* can be calculated as was shown by Jung and Risken [14] for specific boundary conditions and by Risken in a supplement to the second edition of his well-known text book [15] for more general boundary conditions. Using specifically equation (S9.14) from [15] (with $h(v) = \mu(v) - g'(v)g(v)$) together with the symmetry of the functions $\gamma(v)$ and $g(v)$, one obtains

$$D_{\mathrm{eff}} = \frac{\int_0^{v_{\mathrm{M}}} \mathrm{d}v_2\ \mathrm{e}^{U(v_2)} \left[\int_{v_2}^{v_{\mathrm{M}}} \mathrm{d}v_1\ \mathrm{e}^{-U(v_1)} v_1/g^2(v_1)\right]^2}{\int_0^{v_M} \mathrm{d}v_3\ \mathrm{e}^{-U(v_3)}/[mg(v_3)]^2}, \tag{4}$$

where the effective potential reads $U(v) = m^2 \int_0^v \mathrm{d}\tilde{v}\ \mu(\tilde{v})/g^2(\tilde{v})$.

For arbitrary friction and noise functions, the integrals have to be evaluated numerically.

For specific cases (cf sections 3 and 4 below), the integrals can be reduced to higher mathematical functions. We also note that the general structure of the formula resembles exact results for an overdamped BM, namely, the formulae for the diffusion coefficient of an overdamped BM in a periodic force field with additive noise [16, 17] and with spatially periodic noise modulation [18].

It is easily verified from (4) that for $g(v) \equiv \sqrt{\gamma_0 k_{\mathrm{B}} T}$, $\mu(v) = v\gamma_0/m$, $v_{\mathrm{M}} \to \infty$ the formula (4) reproduces the classical result $D_{\mathrm{eff}} = k_{\mathrm{B}}T/\gamma_0$. Further, in cases where the dynamics (1) yields a superdiffusive behaviour [7], our formula diverges (as it is supposed to do for a mean square displacement growing stronger than linear with time). The result (4) can, however, be used to find the values of system parameters at which a transition from normal diffusion to superdiffusion occurs; this will be discussed elsewhere.

We will also confirm the analytical result (4) by numerical simulations of the model (1) as detailed in the appendix.

3. The diffusion coefficient in the case of nonlinear friction

Our first nontrivial example is a nonlinear increase of the friction function as discussed in [4]

$$\gamma(v) = \gamma_0(1 + \alpha v^2), \tag{5}$$

where $\alpha > 0$. This function can also be regarded as a Taylor expansion of a sufficiently smooth and symmetric friction function.

We will assume that the noise strength is given by a generalized Einstein relation [4]

$$g^2(v) = k_B T \gamma(v) \tag{6}$$

and we will interpret the stochastic differential equation (1) in the *kinetic form* (also called Hänggi–Klimontovich interpretation or interpretation in the backward sense). The latter ensures (in contrast to the more common Ito and Stratonovich interpretations of equations with multiplicative noise) that the steady-state density of the velocity will be the Maxwell distribution $\exp[-mv^2/(2k_B T)]$ (see [3, 4]) if and only if the generalized Einstein relation (6) is obeyed. Both the generalized Einstein relation in (6) as well as the usage of the kinetic form of the Fokker–Planck equation has been justified by different derivations from microscopic models (see e.g. [4] and [19] for a more recent example).

The drift term and the effective potential read

$$\mu(v) = \frac{\gamma_0}{m} v[1 + \alpha(v^2 - 2k_B T)], \qquad U(v) = \frac{mv^2}{2k_B T} - \ln(1 + \alpha v^2) \tag{7}$$

and the effective diffusion coefficient can be explicitly calculated from (4)

$$D_{\mathrm{eff}} = \frac{k_B T}{\gamma_0} \sqrt{\pi} z e^{z^2} \operatorname{erfc}(z), \tag{8}$$

where $z = \sqrt{m/(2k_B T\alpha)}$ and erfc (z) is the complementary error function. For $z \gg 1$ this reduces to the result for the linear case $D_{\mathrm{eff}} = k_B T/\gamma_0$ whereas for strong temperature the diffusion coefficient increases sublinearly $D_{\mathrm{eff}} \to \sqrt{m\pi k_B T/(2\alpha\gamma_0^2)}$. In general, the effective diffusion coefficient is always smaller than that in the linear case. Results of simulations show excellent agreement with (8).

Remarkably, although linear and nonlinear BM obey exactly the same velocity (Maxwell) distribution, their diffusion coefficients differ drastically at high temperature. Since $D_{\mathrm{eff}} = \langle v^2 \rangle \tau_{\mathrm{corr}}$ this implies that the velocity correlation time drops with temperature ($\langle v^2 \rangle$ is the same as for linear BM). The stronger dissipation and fluctuations at large speed destroy velocity correlations and thus reduce the velocity's correlation time. We anticipate that a different friction function for which $\gamma(v) < \gamma_0$ for a range of velocities may yield enhanced diffusion compared to the linear case.

4. The diffusion coefficient of a relativistic Brownian particle

Next, we turn to the relativistic BM as recently discussed by Dunkel and Hänggi [5] in terms of equations for position and relativistic momentum. Here the drift and diffusion terms of the velocity have first to be found from a transformation of the Fokker–Planck equation or the Langevin equations to a velocity variable. We use again the kinetic interpretation which in this case ensures that the stationary density coincides with the relativistic Maxwell (or Jüttner) density

$(1-v^2/c^2)^{-3/2}\exp[-mc^2(1-v^2/c^2)^{-1/2}/(k_B T)]$ (see [5]); drift and diffusion in this case read

$$\mu(v) = \frac{\gamma_0 v}{m}\left[(1-v^2/c^2) + \frac{2k_B T}{mc^2}(1-v^2/c^2)^{3/2}\right],$$
$$\frac{g^2(v)}{m^2} = \frac{\gamma_0 k_B T}{m^2}\left(1-\frac{v^2}{c^2}\right)^{5/2}. \tag{9}$$

The diffusion coefficient calculated from the general formula (4) with $v_M = c$ (speed of light) is given by

$$D_{\text{eff}} = \frac{mc^2}{\gamma_0}\left[\beta + \sqrt{\pi}W_{-1/2,1/2}(2\beta)/(2K_0(\beta))\right]^{-1} \tag{10}$$

where $W_{\kappa,\mu}(z)$ and $K_\nu(z)$ denote the Whittaker W function and the modified Bessel function of the second kind [20], respectively, and

$$\beta = \frac{mc^2}{k_B T}, \tag{11}$$

that is, the squared ratio of the speed of light c and the thermal velocity $\sqrt{k_B T/m}$.

For large β the second term in the bracket in (10) approaches zero and we obtain the classical result again. For small β the diffusion coefficient grows only logarithmically $D_{\text{eff}} \sim \ln(k_B T)$. The analytical result from (10) as well as the high-temperature behaviour are confirmed by simulation results shown in figure 2. We note that the simulation results for the diffusion coefficient by Dunkel and Hänggi [5] differ from those presented here because these authors used the Ito interpretation of the Langevin equation instead of the Hänggi–Klimontovich interpretation for the sake of simplicity.

As in the case of nonlinear friction the diffusion coefficient of a relativistic particle is smaller than the classical result (dashed line in figure 2). However, the growth of the diffusion coefficient with temperature is diminished because velocities larger than the speed of light are not possible anymore. In fact, one can show that the correlation time of velocities *increases* with temperature in marked contrast to classical BM (where it is independent of T) and BM with nonlinear friction (where τ_{corr} drops with T). Thus, although the curves in figures 1 and 2 look similar, the dynamical origin of the deviation from the linear case is very different: for the BM with nonlinear friction it was the reduction in velocity correlations while for the relativistic BM it is the limitation in the range of velocities that leads to a diminished diffusion coefficient.

We would like to add two remarks. Firstly, we have restricted ourselves to the kinetic interpretation of the Langevin equation for the relativistic motion. The correct interpretation to be used will depend on the microscopic physics of the BM (the nature of the heat bath and the coupling between Brownian particle and bath). The kinetic interpretation has the important advantage that it yields a Fokker–Planck equation which is satisfied by the Jüttner distribution in the steady-state. Hence, this interpretation corresponds most likely to a broad class of physical systems. However, we cannot exclude that certain systems are more faithfully described by another interpretation of the Langevin equation; for those systems the evaluation of (4) with a modified drift term (corresponding to another interpretation of the Langevin equation) may yield another dependence of the diffusion coefficient on temperature than derived and discussed above. Secondly, the Langevin equations introduced by Dunkel and Hänggi [5] must be regarded as an

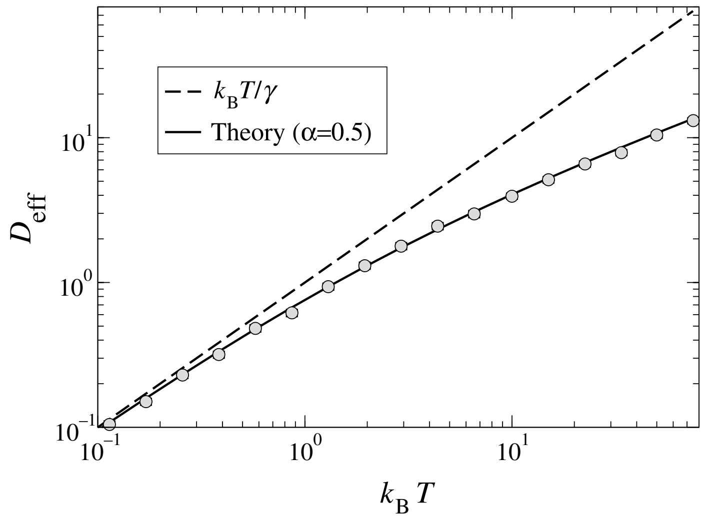

Figure 1. Diffusion coefficient versus temperature for the nonlinear friction function (6) with $\alpha = 0.5$. Theory (8) is given by the solid line; the dashed line shows for comparison the normal diffusion coefficient (no nonlinearity, i.e. $\alpha = 0$). The simulation results (circles) were obtained from 10^3 runs of the dynamics (1) for a time of 2×10^4 with a time step of 10^{-3}. Non-dimensional parameters: $m = 1, \gamma_0 = 1$ and $\alpha = 0.5$. We simulated an Ito equation that corresponds to the *kinetic* form of the Fokker–Planck equation (kinetic interpretation of the original problem, see appendix for details of the simulation).

approximation as pointed out by the same authors in a recent study [19]. From a microscopic binary collision model, Dunkel and Hänggi derived Langevin-like equations which contain a white but non-Gaussian noise. For such a model, the calculation of the diffusion coefficient will be generally much more difficult.

5. The diffusion coefficient of an active Brownian particle

Finally, we apply the formula (4) to a nonequilibrium system, namely, a model of active Brownian particles with energy depot [6, 21]. In this case, the only nonlinearity is in the friction function we have only a nonlinear friction function but a constant noise strength

$$\gamma(v) = \gamma_0\left(1 - \frac{\alpha}{1 + ev^2}\right), \quad g(v) \equiv \sqrt{Q}. \tag{12}$$

The parameter α determines the stability of a finite deterministic velocity: for $Q = 0$ and $\alpha > 1$ there exist two stable velocities $v_0 = \pm\sqrt{(\alpha - 1)/e}$. Accordingly, the steady-state probability density of the noisy system ($Q > 0$) is bimodal for $\alpha > 1$.

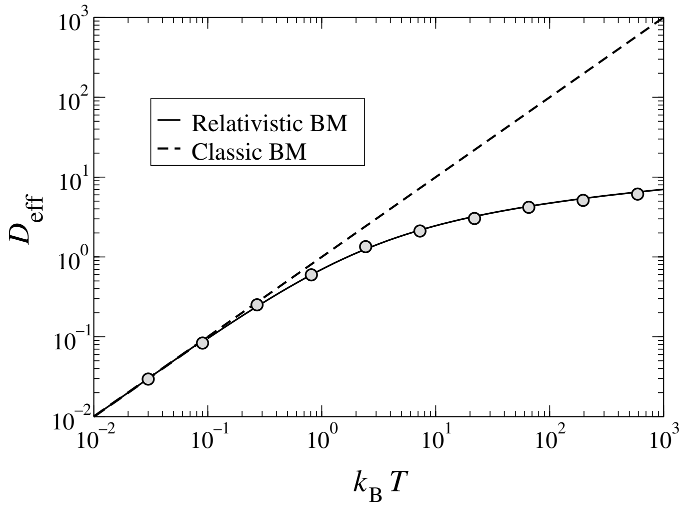

Figure 2. Diffusion coefficient versus temperature for relativistic BM with kinetic interpretation of the Langevin equation. Theory (10) is given by the solid line; the dashed line shows for comparison the normal diffusion coefficient. Nondimensional parameters: $m = 1$, $\gamma_0 = 1$ and $c = 1$. Put differently, the diffusion coefficient and the thermal energy are measured in units of mc^2/γ_0 and mc^2, respectively. We used an Ito stochastic differential equation corresponding to the transport ('kinetic') form of the Fokker–Planck equation (Hänggi–Klimontovich interpretation of the problem) and simulated 10^3 realizations for a time window of 100 unit times with a time step of 10^{-4} (at large noise).

Here we are interested in this bimodal limit and set $\gamma_0 = 20$, $e = 40$ and $\alpha = 10$. The effective velocity potential

$$U(v) = \frac{m\gamma_0}{2Q}\left[v^2 - \frac{\alpha}{e}\ln(1 + ev^2)\right] \tag{13}$$

for this case is shown in the inset of figure 3. It is important to realize that in this nonequilibrium situation negative 'dissipation' ($\gamma(v) < 0$) occurs for low speed and thus, energy is pumped into the system. It is, of course, not possible to balance this negative friction by fluctuations even if we were to allow for a non-constant diffusion coefficient, i.e. if $\gamma(v) < 0$ for some finite range of velocities we are far from thermodynamic equilibrium in any case.

In the nonequilibrium situation the noise intensity Q plays the role played by temperature in the equilibrium system. Analogue to the temperature dependence of the effective diffusion coefficient investigated in the last sections, we will now study the dependence of D_{eff} on the noise intensity Q.

For the system of active BM with (12) we are confined to the numerical evaluation of (4) (the limiting velocity is again $v_M \to \infty$). In figure 3 we show the diffusion coefficient as a function of the noise intensity Q and compare to numerical simulation results. Both theory and stochastic simulations reveal a non-monotonic dependence of the diffusion on the noise intensity—diffusion becomes minimal at a moderate value of $Q \approx 5$ and diverges for both $Q \to 0$ and $Q \to \infty$. In order to understand this remarkable finding, we study the limits of weak and strong noise.

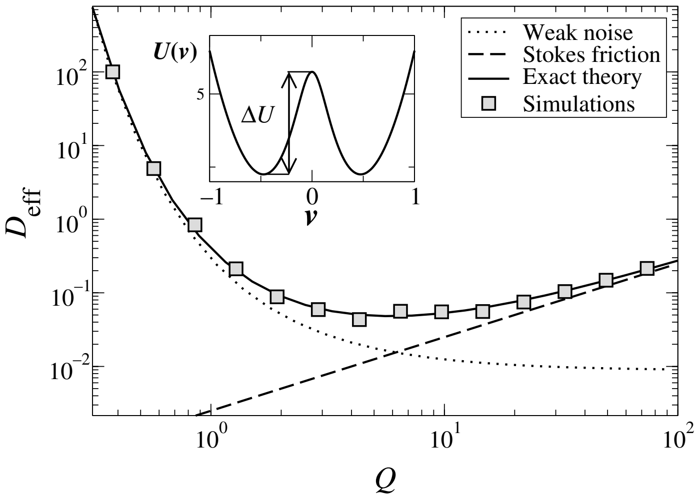

Figure 3. Effective diffusion coefficient of an active Brownian particle with energy depot. Numerical simulation results (symbols) were obtained by integrating (1) with an Euler procedure ($\Delta t = 0.002$) for a time window of $T = 10^4$. From 100 realizations of the mean square displacement, we estimated the diffusion coefficient. The quadrature formula (solid line) was obtained using the computer program MAPLE; shown are also the weak and strong noise approximations (14) and (15), respectively. Inset: velocity potential for a Brownian particle with energy depot (cf (12)) for the parameters used in the text and $Q = 1$.

For weak noise, a standard saddle-point approximation of (4) yields for $\Delta U = m\gamma_0[1 + \alpha(\ln(\alpha) - 1)]/(2Qe) \gg 1$

$$D_{\text{eff}} \approx \frac{v_0^2 \pi}{Q\sqrt{U''(v_0)|U''(0)|}} \exp\left[\Delta U\right] = \frac{v_0^2}{2r_{\text{K}}}, \tag{14}$$

where r_{K} is the well-known Kramers rate for the escape from one of the potential minima over the barrier at $v = 0$ in the overdamped case (in this calculation, v is regarded as the position variable of an overdamped particle subject to white noise and the potential $U(v)$). At small noise the velocity is essentially either at v_0 or at $-v_0$ and switches between these values with the rate r_{K}. The active particle has in this limit a velocity corresponding to a telegraph noise. The diffusion coefficient of such a particle has been known for a long time (see e.g. [22]). Remarkably, at weak noise the diffusion coefficient *drops* with increasing noise and diverges for vanishing noise. For $Q \to 0$, half of the particles of an ensemble would have velocity v_0 and the other half $-v_0$, yielding in total a ballistic increase in mean square displacement. This is reflected in the divergence of the diffusion coefficient for vanishing noise.

At large noise, the barrier becomes irrelevant and the particle feels only the extreme parts (i.e. at $|v| \to \infty$) of the potential, which means that we obtain in this limit normal Brownian diffusion, i.e. for $\Delta U \ll 1$ we obtain

$$D_{\text{eff}} \approx Q/\gamma_0^2 \tag{15}$$

which, of course, increases with growing noise intensity.

From the two limits it is evident that the diffusion coefficient attains at least one minimum for $\Delta U(Q) \sim 1$. Naturally, the minimal diffusion coefficient is still larger than that of a passive particle ($\alpha = 0$).

If we assume that the noise intensity is an accessible parameter, we can localize the active particle, i.e. constrain the particle to a certain area of size L by driving the particle with a noise of intensity $Q_{\rm min}$. This will work, of course, only for times much smaller than $L^2/D_{\rm eff}(Q_{\rm min})$.

A minimum in the effective diffusion coefficient is also expected for higher spatial dimensions. As shown by different authors [23]–[25], in 2D for instance, the diffusion coefficient drops at weak noise like Q^{-1}. It increases at large noise for the very same reason as given above for the one-dimensional system. Thus, our general conclusion is that for active Brownian particles, diffusion is minimized by a finite amount of fluctuation. One may speculate here about a constructive role of noise: self-propelled motion without fluctuations leads to ballistic motion and may be suboptimal in a search for food or other tasks that may require to cover exhaustively a certain area (see also [24] which deals with this issue for the related problem of Daphnia swarming).

6. Summary and conclusions

We have derived a formula for the diffusion coefficient of nonlinear BM in one spatial dimension and discussed three distinct applications. We saw that in equilibrium systems where friction and fluctuations increase strongly at high speeds, the diffusion coefficient is reduced compared to the case of Stokes' friction. This reduction is caused by a reduction in velocity correlation time. We found furthermore that a relativistic particle also exhibits reduced diffusion, however, for a completely different reason: the support of possible velocities ($|v| < c$) sets an upper limit for the velocity variance ($\langle v^2\rangle < c^2$) which therefore cannot grow unbounded as for linear BM. The remaining logarithmic growth in the diffusion coefficient with temperature is thus due to an *increase in correlation time with growing temperature* which stands in marked contrast to both cases of linear BM and nonlinear friction. Finally, we also uncovered a simple yet remarkable noise-induced effect in a nonequilibrium model of self-propelled motion: diffusion is minimized at a finite strength of the driving noise. This remarkable effect holds true in higher dimensions and may have implications for optimal strategies in searching for spatially distributed food sources.

The analytical result (4) could be also used to explore other issues, for instance, (i) a non-monotonic friction function $\gamma(v)$ in an equilibrium system leading possibly to enhanced diffusion; (ii) nonlinear friction functions in the relativistic case (Stokes' law is not valid at high speed regardless of relativistic effects); (iii) active BM in which the noise intensity is a function of velocity too, modelling more general mechanisms of self-propelled activity. A particularly interesting application which we did not address in this paper is the occurrence of superdiffusion in the model (1) for certain friction and noise functions [7]. For such systems, the quadrature expression will diverge for parameters that result in superdiffusion—hence the analytical result can be used to determine parameter regimes of superdiffusion. This problem will be addressed in a forthcoming publication.

Appendix

Here we explain how to simulate the dynamics (1) corresponding to the kinetic interpretation of the Langevin equation and how to measure the effective diffusion coefficient.

The kinetic interpretation corresponds to the so-called postpoint-discretization rule. This implies that we take the velocity in the multiplicative noise term at the end of the interval leading to an implicit Euler integration scheme as follows

$$x(t+\Delta t) = x(t) + v(t)\Delta t, \tag{A.1}$$

$$v(t+\Delta t) = v(t) - \frac{\gamma(v(t))}{m} v(t)\Delta t + \frac{g(v(t+\Delta t))}{m}\sqrt{2\Delta t}a_{\mathrm{i}}, \tag{A.2}$$

where the a_{i} is a sequence of independent Gaussian random numbers with zero mean and unit variance. In lowest order this implicit scheme corresponds to an explicit Euler scheme

$$x(t+\Delta t) = x(t) + v(t)\Delta t, \tag{A.3}$$

$$v(t+\Delta t) = v(t) - \left[\frac{\gamma(v(t))}{m} v(t) - 2\frac{g(v(t))g'(v(t))}{m^2}\right]\Delta t + \frac{g(v(t))}{m}\sqrt{2\Delta t}a_{\mathrm{i}}, \tag{A.4}$$

where $g'(v) = \mathrm{d}g/\mathrm{d}v$ is the derivative of g with respect to v. In other words, the original equation (1) interpreted in the kinetic sense corresponds to the equation

$$m\dot{v} = -\gamma(v)v + 2g(v)g'(v)/m + g(v)\xi(t) \tag{A.5}$$

interpreted in the Ito sense. For a similar equivalence between Ito and Stratonovich interpreted equations see [26], section 4.3.6.

From N realizations $x_i(t)$ $(i = 1, \ldots, N)$ of the process simulated in a time window $t \in (0, T)$ with initial condition $x_i(0) = 0$, we can estimate the mean square displacement $\langle (x(T) - \langle x(T)\rangle)^2\rangle = \langle x(T)^2\rangle - \langle x(T)\rangle^2$ by means of the first two moments $\langle x(T)\rangle = (1/N)\sum_{i=1}^{N} x_i(T)$ and $\langle x(T)^2\rangle = (1/N)\sum_{i=1}^{N} x_i^2(T)$. From the mean square displacement the diffusion coefficient can be estimated by $D_{\mathrm{eff}} = \langle (x(T) - \langle x(T)\rangle)^2\rangle/(2T)$.

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