Heavy-Tail Phenomena in Homogenized Models of Brownian Particle in Active Heat Bath

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ABSTRACT

In these notes, we study stochastic models describing a (passive) Brownian particle interacting with an active heat bath. The active heat bath is modeled by a non-Gaussian process capturing a particular self-propelled motion of the particle. This is in contrast to the passive bath, which is modeled effectively by a (Gaussian) Ornstein-Uhlenbeck process. From these models, we identify relevant time scale separation and derive homogenized models in the limit of infinite time scale separation. The homogenized models are described by SDEs which may include effective drift terms. We further study stationary distributions of these SDEs. We find that, in contrast to the case of passive bath, the stationary distributions of the SDEs are generally non-Gaussian and, in particular, exhibit activity-induced heavy tails.

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1 General Model

Consider

$$\frac{d\mathbf{q}(t)}{dt} = \mathbf{u}(t) + \mathbf{F}(\mathbf{q}(t)) + \boldsymbol{\sigma}\boldsymbol{\xi}(t), \tag{1}$$

where $u(t) \in \mathbb{R}^n$ is a random velocity process (for instance, functional of a Wiener process), $F : \mathbb{R}^n \to \mathbb{R}^n$ is a (deterministic) external force, $\xi \in \mathbb{R}^k$ is a Gaussian white noise and $\sigma : \mathbb{R}^k \to \mathbb{R}^n$ is a constant matrix. The initial condition is q(0) = q (independent of $\{\xi(t), u(t), t \geq 0\}$), and ξ and u are independent processes.

2 Stochastic Model for a Trapped Passive Brownian Particle in an Active Bath

2.1 1D Model

Consider the following Langevin model (in the form of eqn. (5) in [2]) for position, $x \in \mathbb{R}$, of a trapped passive Brownian particle in an active bath:

$$\frac{dx}{dt} = -\frac{1}{\gamma} \frac{dV(x)}{dx} + \eta_p + \eta_a, \tag{2}$$

where $\gamma>0$ is the particle friction coefficient, V(x) is the potential, η_p represents the thermal Gaussian (white) noise characterized by $\langle \eta_p(t+\tau)\eta_p(t)\rangle=2D_T\delta(\tau)$ (recall that D_T is the translational diffusion coefficient and is related to γ by the fluctuation-dissipation relation $D_T\gamma=k_BT$), and η_a represents the fluctuations due to the presence of the active bath.

We take the potential to be harmonic, i.e. $V(x) = \frac{1}{2}kx^2$, with stiffness k > 0. We are going to write (2) as a SDE in a differential form. To this end, we write $\eta_p dt = \sqrt{2D_T} dW_t^T$, where W_t^T is a Wiener process, i.e. a mean zero Gaussian process with $\langle W_t^T W_s^T \rangle = \min(t,s)$ [11]. In the literature, there are various self-propulsion models, falling under the name of run-and-tumble particles, active Brownian particles and active Ornstein-Uhlenbeck particles [5, 13]. We model η_a as the following non-Gaussian process:

$$\eta_a = v_0 \cos(\phi_t),\tag{3}$$

where $v_0 > 0$ is a constant and ϕ solves the SDE:

$$d\phi_t = \sqrt{2D_R} dW_t^R, \tag{4}$$

where D_R is the rotational diffusion coefficient and W_t^R is a Wiener process independent of W_t^T .

The above considerations allow us to rewrite (2) in the form of Itô SDEs for the position process x_t and angle process ϕ_t :

$$dx_t = -\frac{k}{\gamma} x_t dt + \sqrt{2D_T} dW_t^T + v_0 \cos(\phi_t) dt, \tag{5}$$

$$d\phi_t = \sqrt{2D_R} dW_t^R. (6)$$

The initial conditions are taken to be as follows: $x_0 = x$ (which can be random or simply a constant) and ϕ_0 is a random variable uniformly distributed on $[0, 2\pi]$, i.e. $\phi_0 \sim \text{Unif}[0, 2\pi]$.

Two important length scales are the persistence length, $L_a=\frac{v_0}{D_R}$, associated with the active bath and the characteristic dimension, $L_{ot}=\sqrt{\frac{k_BT}{k}}$, of the harmonic trap (width of the Gaussian distribution proportional to $e^{-V(x)/k_BT}$). On the other hand, two important time scales are the rotational diffusion time, $\tau_R \propto 1/D_R$, and the time, $\tau_{ot}=\gamma/k$, needed by the particle to move to the center of the harmonic trap. We are going to demonstrate, using a simplifying assumption, how interplay between these two length scales or time scales could lead to transition of stationary position probability distribution from a Boltzmann to a non-Boltzmann regime, and to quantify the deviation from a Boltzmann description.

The simplifying assumption is that D_R is small enough to be neglected (or $\tau_R \gg \tau_{ot}$ or $L_a \gg L_{ot}$). In view of the conclusion in [2], we expect non-Boltzmann statistics to emerge. This assumption implies that $\phi_t = \phi_0 + \sqrt{2D_R}W_t^R = \phi_0 \sim \text{Unif}[0,2\pi]$ for all $t \geq 0$. Physically, this means that the self-propelled particles making up the active bath are equally likely to explore all possible directions in space at any given time point – this is not an unrealistic assumption afterall. Writing down the Fokker-Planck equation and solving for the stationary probability distribution (see Appendix A for details), one finds that:

$$P_{st}(x,\phi) = C_1 \exp\left(-\frac{k}{2D_T \gamma}x^2 + \frac{v_0}{D_T}\cos(\phi)x\right),\tag{7}$$

where C_1 is a normalization constant. Therefore,

$$P_{st}(x) = \frac{1}{2\pi} \int_0^{2\pi} P_{st}(x,\phi) d\phi = C_1 \exp\left(-\frac{k}{2D_T \gamma} x^2\right) I_0\left(\frac{v_0}{D_T} x\right)$$
(8)

$$=: C_1 \exp\left(-\frac{V_b(x)}{k_B T}\right) I_0\left(\frac{V_a(x)}{k_B T}\right),\tag{9}$$

where I_0 denotes the 0th-order modified Bessel function of the first kind (note: $I_0(0) = 1$), $V_b(x) = V(x)$ and $V_a(x) = \gamma v_0 x$ (note that we have made use of the fluctuation-dissipation relation $D_T \gamma = k_B T$).

The presence of the multiplicative factor in the form of I_0 makes the stationary distribution to have heavy tails. In particular, the ratio $v_0/D_T=v_0\gamma/(k_BT)$ serves as a useful parameter to quantify the deviation of the distribution from a Boltzmann one: the greater the deviation of v_0 from zero, the more heavier the tails of the distribution. Increasing v_0 past the critical value $v_c=\sqrt{\frac{2kD_T}{\gamma}}$, the stationary distribution exhibits double peaks (i.e. it is symmetric and bi-modal, with a local minimum at the origin), illustrating dominance of the active fluctuations which steer the particle away from the trap center in the long run. This result also qualitatively agrees with the findings of the model of a trapped active particle in a passive bath [12, 3, 16].

Let us end this section with a remark. In [2], q-Gaussian distributions are used to fit the observed distributions which exhibit heavy tails. To our knowledge, stationary distributions of a q-Gaussian form are natural for a class of SDEs driven by a sum of additive and multiplicative noise [1]. An example is the following Itô SDE:

$$dx_t = -\frac{k}{\gamma} x_t dt + \sqrt{2D_T} dW_t^T + \sigma x_t dW_t^k, \tag{10}$$

where $\sigma>0$ is a constant, and W_t^T and W_t^k are independent Wiener processes. Although the above SDE can be obtained from (5) by setting $v_0=0$ and replacing k by $k+\xi_t$, where $\xi_t=-\gamma\sigma\frac{dW_t^k}{dt}$, it does not seem to be a sensible model for a Brownian particle in an active bath.

2.2 2D Model

Taking the trapping potential to be harmonic and symmetric, i.e. $V(x,y) = \frac{1}{2}k(x^2 + y^2) = V(x)V(y)$, we consider the following SDEs for the position process $(x_t, y_t) \in \mathbb{R}^2$ and angle process $(\phi_t^1, \phi_t^2) \in \mathbb{R}^2$:

$$dx_{t} = -\frac{k}{\gamma}x_{t}dt + \sqrt{2D_{T}}dW_{t}^{T,1} + v_{0}\cos(\phi_{t}^{1})dt,$$
(11)

$$dy_t = -\frac{k}{\gamma} y_t dt + \sqrt{2D_T} dW_t^{T,2} + v_0 \sin(\phi_t^2) dt,$$
(12)

$$d\phi_t^1 = \sqrt{2D_R} dW_t^{R,1},\tag{13}$$

$$d\phi_t^2 = \sqrt{2D_R} dW_t^{R,2},\tag{14}$$

where the Wiener processes $W_t^{T,1}$, $W_t^{T,2}$, $W_t^{R,1}$ and $W_t^{R,2}$ are independent. The initial conditions are taken to be as follows: $x_0 = x$, $y_0 = y$ (which can be random or simply a constant), and ϕ_0^1 and ϕ_0^2 are independent random variables uniformly distributed on $[0,2\pi]$. The fact that ϕ_0^1 and ϕ_0^2 are independent random variables, instead of the same random variable, is important to distinguish the model of a passive Brownian particle in an active bath from that of an active particle in a passive bath [4, 15].

We again assume that D_R is negligible as in the 1D case. Under this assumption, one can compute the stationary probability distribution:

$$P_{st}(x,y) = C_2 \exp\left(-\frac{k}{2D_T \gamma}(x^2 + y^2)\right) I_0\left(\frac{v_0}{D_T}x\right) I_0\left(\frac{v_0}{D_T}y\right)$$
(15)

$$=: C_2 \exp\left(-\frac{V_b(x) + V_b(y)}{k_B T}\right) I_0\left(\frac{V_a(x)}{k_B T}\right) I_0\left(\frac{V_a(y)}{k_B T}\right), \tag{16}$$

where C_2 is a normalization constant, and V_b and V_a are as before.

On the other hand, repeating the derivation for the model of an active particle in a passive bath, in which case $\phi_0^1 = \phi_0^2 = \phi_0 \sim \text{Unif}[0, 2\pi]$, with $D_R = 0$, one finds that the stationary probability distribution is given by:

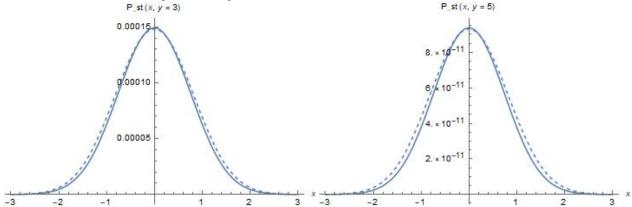
$$P'_{st}(x,y) = C_3 \exp\left(-\frac{k}{2D_T \gamma}(x^2 + y^2)\right) I_0\left(\frac{v_0}{D_T} \sqrt{x^2 + y^2}\right),\tag{17}$$

where C_3 is a normalization constant. Note that $P'_{st}(x,y) \neq P_{st}(x,y)$ and in fact it has, in general, slightly heavier tails than that of $P_{st}(x,y)$ (see Figure 1). However, the critical values of v_0 beyond which the distribution becomes bi-modal are the same for the two models – it is $v_c = \sqrt{\frac{2kD_T}{\gamma}}$, due to the symmetry and close resemblance of our 2D model to the 1D one. The difference in the stationary distribution illustrates the different nature of the two models. Although one expects passive particle in an active bath to qualitatively behave like an active particle due to multiple interactions with the self-propelled particles, there are notable quantitative differences even in the long time limit.

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Figure 1: Plots of stationary position probability distribution at y=3 (left) and y=5 (right) for two different 2D models: the dashed line corresponds to the stationary distribution for the model of passive particle in an active bath and the solid line to that of active particle in a passive bath.



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Appendices

A Fokker-Planck Equation and Probability Distribution

We first consider the 1D model in the following. The Fokker-Planck equation (or forward Kolmogorov equation), associated with (5)-(6), for the probability distribution of the process (x_t, ϕ_t) is:

$$\frac{dP(x,\phi,t)}{dt} = \frac{k}{\gamma} \frac{\partial}{\partial x} (xP) + v_0 \cos(\phi) \frac{\partial P}{\partial x} + D_T \frac{\partial^2 P}{\partial x^2} + D_R \frac{\partial^2 P}{\partial \phi^2}.$$
 (18)

One could, in principle, solve the above PDE using the Fourier transform method as in [14] but the resulting solution is obtained in a form of series expansion which does not allow convenient analysis of the probability distribution unless further assumptions are made. Under our assumption that $D_R = 0$, the stationary probability distribution (8) follows by setting the right hand side in the above equation to zero and solving for P.

We now derive the probability distribution P(x, t) of the particle's position for all time t. The solution to the SDEs (5)-(6) can be written as:

$$x_{t} = x_{0}e^{-\frac{k}{\gamma}t} + \sqrt{2D_{T}} \int_{0}^{t} e^{-\frac{k}{\gamma}(t-s)} dW_{s}^{T} + v_{0} \int_{0}^{t} e^{-\frac{k}{\gamma}(t-s)} \cos(\phi_{0} + \sqrt{2D_{R}}W_{s}^{R}) ds, \tag{19}$$

which is clearly non-Gaussian, subjecting to non-Gaussian perturbation introduced by the last integral term above. Note that $\langle |x_t| \rangle \leq \langle |x_0| \rangle + \frac{v_0 \gamma}{k}$ and so we expect the particle to be confined, on average, within a distance of $v_0 \gamma/k$ from its initial position.

We are going to set $D_R = 0$ in the following to simplify the analysis, in which case:

$$dx_t = -\frac{k}{\gamma} x_t dt + v_0 f(\phi_0) dt + \sqrt{2D_T} dW_t^T = : -\frac{\partial}{\partial x} U^{eff}(x_t, \phi_0) dt + \sqrt{2D_T} dW_t^T, \tag{20}$$

where $U^{eff}(x,\phi) = \frac{k}{2\gamma}x^2 - v_0\cos(\phi)x$ and

$$f(\phi_0) = \cos(\phi_0),\tag{21}$$

which can be interpreted as a random external forcing added to the system that otherwise could be described by an Ornstein-Uhlenbeck process. Here, $\phi_0 \sim \text{Unif}[0, 2\pi]$.

Taking the initial condition $x_0 = y$, where y is a constant, the conditional probability distribution of x_t given ϕ_0 can be shown to be:

$$P(x,t|\phi_0) = \sqrt{\frac{\mu}{2\pi D_T (1 - e^{-2\mu t})}} \exp\left(-\frac{\mu \left(x - y e^{-\mu t} - \frac{v_0}{\mu} (1 - e^{-\mu t}) f(\phi_0)\right)^2}{2D_T (1 - e^{-2\mu t})}\right),\tag{22}$$

where $\mu = k/\gamma$. Therefore, the probability distribution of x_t is given by:

$$P(x,t) = \frac{1}{2\pi} \int_0^{2\pi} P(x,t|\phi_0 = \phi) d\phi.$$
 (23)

A rewriting gives:

$$P(x,t) = \sqrt{\frac{\mu}{2\pi D_T (1 - e^{-2\mu t})}} \exp\left(-\frac{\mu (x - ye^{-\mu t})^2}{2D_T (1 - e^{-2\mu t})}\right) Q(x,t), \tag{24}$$

where

$$Q(x,t) = \frac{1}{2\pi} \int_0^{2\pi} \exp\left(\frac{2v_0(x - ye^{-\mu t})(1 - e^{-\mu t})\cos(\phi) - \frac{v_0^2}{\mu}(1 - e^{-\mu t})^2\cos^2(\phi)}{2D_T(1 - e^{-2\mu t})}\right) d\phi.$$
 (25)

Formula (24) is the main result of this appendix. Note that if $v_0=0$, then Q(x,t)=1, in which case P(x,t) is simply the probability distribution of an Ornstein-Uhlenbeck process modeling the position of a Brownian particle in a passive bath. The addition of the active bath (i.e. $v_0\neq 0$) gives rise to the multiplicative factor Q(x,t) and leads to non-Boltzmann stationary distribution. Formula (24) also gives an alternative way to derive the stationary distribution in (8) by sending $t\to\infty$ in (24).

The above derivations can be repeated to study the 2D model, under the assumptions used in Section 2.2. Let $z_t = (x_t, y_t) \in \mathbb{R}^2$ and cast (11)-(14) as:

$$dz_t = -\nabla_z U(z_t)dt + v_0 n_t dt + \sqrt{2D_T} dW_t^T,$$
(26)

where U(z)=V(x,y) is a harmonic symmetric potential, $\boldsymbol{n}_t=(\cos(\phi_0^1+\sqrt{2D_R}W_t^{R,1}),\sin(\phi_0^2+\sqrt{2D_R}W_t^{R,2}))$, and $\boldsymbol{W}_t^T=(W_t^{T,1},W_t^{T,2})$. Note that when $\phi_0^1=\phi_0^2=0$ and $W_t^{R,1}=W_t^{R,2},$ \boldsymbol{n}_t is simply a Wiener process on a unit circle, which is exponentially ergodic and has the uniform measure as its invariant distribution [8, 7].

Setting $D_R = 0$, we can rewrite the above SDE as:

$$d\boldsymbol{z}_{t} = -\nabla_{\boldsymbol{z}}U(\boldsymbol{z}_{t})dt + v_{0}\boldsymbol{n}(\boldsymbol{\phi}_{0})dt + \sqrt{2D_{T}}d\boldsymbol{W}_{t}^{T} =: -\nabla_{\boldsymbol{z}}U^{eff}(\boldsymbol{z}_{t}; \boldsymbol{\phi}_{0})dt + \sqrt{2D_{T}}d\boldsymbol{W}_{t}^{T},$$
(27)

where
$$U(\boldsymbol{z}) = V(x,y)$$
, $\boldsymbol{n}(\phi_0) = (\cos(\phi_0^1), \sin(\phi_0^2))$, $\boldsymbol{W}_t^T = (W_t^{T,1}, W_t^{T,2})$, and $U^{eff}(\boldsymbol{z}; \boldsymbol{\phi}) = \frac{k}{2\gamma} |\boldsymbol{z}|^2 - v_0 \boldsymbol{n}(\boldsymbol{\phi}) \cdot \boldsymbol{z}$.

The conditional stationary probability distribution is $P_{st}(z|\phi_0) = Ce^{-U^{eff}(z;\phi_0)}$, where C is a normalization constant, and so the stationary probability distribution for the particle's position in the 2D case is $P_{st}(z) = \frac{C}{(2\pi)^2} \int_0^{2\pi} d\phi_2 \int_0^{2\pi} d\phi_1 e^{-U^{eff}(z;\phi)}$, giving the formula (15). Alternatively, since U^{eff} is at most quadratic in z, one could write down the full probability distribution of z_t for all t. Taking $t \to \infty$ in the expression for the probability distribution then gives (15). In the 2D case, one could also work in the polar coordinates but one expects to derive the same results.

B Pathwise Asymptotic Behavior of the Position Process

We restrict our study to the 1D model. Extension to the 2D model is straightforward. We set $\sqrt{2D_R} = \epsilon \sqrt{2D}$, where D>0 is a constant and $\epsilon>0$ is a small parameter, in the SDEs (5)- (6), in which case the solution, x_t^{ϵ} , to the resulting SDEs reads:

$$x_t^{\epsilon} = xe^{-\frac{k}{\gamma}t} + \sqrt{2D_T} \int_0^t e^{-\frac{k}{\gamma}(t-s)} dW_s^T + v_0 \int_0^t e^{-\frac{k}{\gamma}(t-s)} \cos(\phi_0 + \epsilon\sqrt{2D}W_s^R) ds, \tag{28}$$

where $x_0^{\epsilon} = x_0 = x$ and $t \geq 0$.

The mean-squared displacement, two-time correlation function and various moments, such as skewness and kurtosis, of x_t^{ϵ} can be derived for arbitrary $\epsilon > 0$ using Itô stochastic calculus. Here we focus on the asymptotic behavior of x_t^{ϵ} for small ϵ . Using stochastic Taylor expansion, one has:

$$\cos(\phi_0 + \epsilon \sqrt{2D}W_s^R) = \cos(\phi_0) - \epsilon \sin(\phi_0)\sqrt{2D}W_s^R - \epsilon^2 \cos(\phi_0)D(W_s^R)^2 + O(\epsilon^3). \tag{29}$$

In the following, E[.] denotes mathematical expectation.

Proposition 1. The family of processes x_t^{ϵ} converge to x_t , solving the SDE (5) with $\phi_t = \phi_0 \sim \text{Unif}[0, 2\pi]$, in the limit as $\epsilon \to 0$, in the following sense: for all p > 0 and T > 0, $E[\sup_{t \in [0,T]} |x_t^{\epsilon} - x_t|^p] = O(\epsilon^p)$ as $\epsilon \to 0$.

We refer to [10, 9] for other types of limiting procedure studied in the context of active Brownian motion. We end this appendix with a few remarks.

If, in addition to the above, we also set $\sqrt{2D_T} = \epsilon \sqrt{2D'}$, then the SDEs (5)-(6) correspond to a stochastic dynamical system perturbed by a small noise. One could then use the large deviation theory of Freidlin-Wentzell [17] to study rigorously the behavior of such system for small ϵ .

The opposite limit of $D_R \to \infty$ can also be studied, in which case the asymptotic stationary distribution of position is, to the zeroth order, a Boltzmann distribution. This limit is not interesting from the point of view of the experimental results obtained in [2].

Various generalizations of the model studied here or comparison to other models can also be considered. For instance, the case where the potential is asymmetric or is a symmetric double-well, the case where v_0 is state-dependent, the case where chirality of the active particles is introduced, the case where the particle moves in the presence of obstacles and boundaries, etc.

For instance, in the 1D model where the potential is a symmetric double-well and the self-propelled particles in the active bath are chiral (in which case ϕ_t also rotates with an angular frequency Ω), it is expected that stochastic resonance [6], a phenomenon that manifests itself by a synchronization of activated hopping events between the potential minima with the periodic forcing, $f(t, \phi_0) = \cos(\phi_0 + \Omega t)$, introduced by the active fluctuations, will occur (here we set $D_R = 0$), leading to the amplification of the weak forcing (for small v_0).