Non-Equilibrium Stat. Mech.

Project 2
Stochastic differential equations with memory

The aim of this project is to study by means of numerical simulations the stochastic dynamics of a random walker, described by Langevin equations, in the presence of Non-Marvokian noise. The general starting point will be

$$\gamma\dot{\mathbf{r}}(t) = \mathbf{F}(\mathbf{r}) + \boldsymbol{\xi}(t) \tag{1}$$

where $\boldsymbol{\xi}$ is a Gaussian noise verifying

$$\langle\boldsymbol{\xi}\rangle_n = \mathbf{0}, \;\; \langle\xi_\alpha(t)\xi_\beta(t')\rangle_n = \Gamma(t-t')\delta_{\alpha\beta} \tag{2}$$

The brackets $\langle\rangle_n$ denote averages over the noise distribution.

Such dynamics mimics the presence of some memory in the motion of the walker. Memory is generically present in any physical problem but usually disregarded if the time scales involved are much smaller that the ones of interest. In many situations, the correlation time of the noise can be of the same order of magnitude as the relevant slow variables in the problem. In these cases, memory, in the form of a colored noise, should in principle be taken into account. Here we will consider a simple model system to illustrate it.

We consider N persistent Brownian walkers, moving in a 2D $L \times L$ box, governed by the following set of overdamped Langevin equations [2]

$$\gamma\dot{\mathbf{r}}_i(t) = \mathbf{F}_i + \boldsymbol{\xi}_i \tag{3}$$

$$\dot{\boldsymbol{\xi}}_i(t) = -\frac{\boldsymbol{\xi}_i}{\tau} + \sqrt{\frac{2D}{\tau^2}}\boldsymbol{\eta}_i(t) \tag{4}$$

Here $\boldsymbol{\xi}_i$ is a Non-Markovian noise, described by an *Ornstein-Uhlenbeck process* with characteristic persistence or correlation time τ. On the contrary, $\boldsymbol{\eta}_i$ is a Gaussian white noise of zero mean and unit variance. Such noise introduces persistence in the spatio-temporal dynamics of the Brownian particles via the autocorrelation function

$$\langle\boldsymbol{\xi}_i(t)\boldsymbol{\xi}_j(t')\rangle = \frac{D}{\tau}e^{-|t-t'|/\tau}\delta_{ij}\mathbf{1} \tag{5}$$

This model is typically used to describe self-propelled particles, and reduces to passive (equilibrium) Brownian motion in the limit $\tau \to 0$, for which $\langle\boldsymbol{\xi}_i(t)\boldsymbol{\xi}_j(t')\rangle \to 2D\delta(t-t')\delta_{ij}\mathbf{1}$ (in the distribution sense). From now on, we fix $\gamma = 1$.

1. Discretise eq. 3 using the Euler-Mayurama scheme. Implement periodic boundary conditions (PBC). Explain your criteria to choose the different simulation parameters, N, L, D, and in particular, the time step and the total simulation run time.
2. Compute the MSD of free ($\mathbf{F}_i = 0$) particles for several parameters τ and compare with

$$\Delta^2(t) = 4D(t + \tau(e^{-t/\tau} - 1)) \tag{6}$$

Describe the motion of the particles and plot a typical trajectory for $\tau = 1, 10, 100$. Specify clearly the value of all the simulation parameters.

3. Compute the correlation function

$$N^{-1} \sum_i \langle \boldsymbol{\xi}_i(t) \boldsymbol{\xi}_i(t') \rangle$$

for $\tau = 1, 10, 100$ and check that, indeed it decays exponentially fast with a characteristic time given by τ.

4. Apply a constant force along a given axis, denoted Ox: $\boldsymbol{f}_i = \epsilon_i f \boldsymbol{u}_x$, where $\epsilon_i = \pm 1$ with equal probability. Plot the MSD along x

$$\Delta_x^2(t) = N^{-1} \sum_i \langle (x_i(t) - x_i(0))^2 \rangle$$

and the displacement

$$d_x(t) = N^{-1} \sum_i \epsilon_i \langle x_i(t) - x_i(0) \rangle$$

for non-interacting particles, using $\tau = 10$ and $f = 0,\ 0.001,\ 0.01, 0.1, 1$ (Show them in log-log in two separate plots). Average over, at least 10 independent noise realizations. For which value of f can we consider the force as a perturbation? Do we reach the linear response regime?

5. Use the previous results to measure

$$\mu = \lim_{t \to \infty} \frac{d_x}{ft}$$

and

$$D = \lim_{t \to \infty} \frac{\Delta_x^2(t)}{2t}$$

for several values of τ. Plot μ and D vs τ.

6. (bonus) Consider the particles in a 1D harmonic potential centred in $x_0 = L/2$: $\boldsymbol{F}_i = -\nabla_i U$ with $U = \frac{1}{2}k(x_0 - x_i)^2$. Again, apply a constant force $\boldsymbol{f}_i = \epsilon_i f \boldsymbol{u}_x$, measure μ and D in the linear regime for several values of τ. Show that the Stokes-Einstein relation is violated but can be recovered in terms of an effective temperature which depends on the potential stiffness:

$$T_{eff}/T = 1/(1 + \tau k \mu) \tag{7}$$

7. (bonus) Conclusion: Discuss the non-equilibrium nature of the system (if any).

References

[1] J. Garcia-Ojalvo, J. M. Sancho, and L Ramirez-Piscina. *Generation of spatiotemporal colored noise.* Phys. Rev. A 46, 4670, 1992.

[2] G. Szamel, *Self-propelled particle in an external potential: Existence of an effective temperature*, Phys. Rev. E, **90**, 12111, 2014.

[3] D. Martin, J. O'Byrne, M. E. Cates, E. Fodor , C. Nardini, J. Tailleur and F. van Wijland, *Statistical mechanics of active ornstein uhlenbeck particles*, Phys. Rev. E, **103**, 032607, 2021.