Exercises : Stochastic thermodynamics & Non-equilibrium statistical mechanics

1

Consider the following Lagevin equations :

$$\dot{x} = \sqrt{2D}\zeta(t)\,, \tag{1}$$
$$\dot{x} = f + \sqrt{2D}\zeta(t)\,, \tag{2}$$
$$\dot{x} = k(x_0 - x) + \sqrt{2D}\zeta(t)\,, \tag{3}$$

where $\zeta(t)$ is a delta-correlated noise and D, k and f are constants. Assume that the dynamics occurs in a domain $[-L, L]$ with periodic boundary conditions. Simulate the Langevin equations and obtain from the simulations $p(x,t)$. Calculate the associated Fokker-Planck equations and compare with simulations. What can you say regarding $\langle x \rangle$ and $\langle x^2 \rangle$.Connect the obtained results to a particle immersed in a thermal bath at temperature T. What is the relation between D and T ?

2

Consider the following Lagevin equation :

$$\dot{x} = -\partial_x U\sqrt{2D}\zeta(t)\,, \tag{4}$$
$$\tag{5}$$

where $\zeta(t)$ is a delta-correlated noise and $U = x^4 - \frac{1}{2}x^3 - \frac{3}{2}x^2$. Start with an ensemble of particles at $x = -0.69859$. Where do you expect to find the particles for $t \to \infty$? Compute the rate at which particles move to the global minimum. Compare with the theory.

3

Simulate a system of N non-interacting self-propelled particles moving on a two-dimensional space. Assume periodic boundary conditions. The equation of motion of the i-th particle is given by :

$$\dot{\mathbf{x}}_i = v_0(\cos(\theta_i), \sin(\theta_i)) \tag{6}$$
$$\dot{\theta}_i = \sqrt{2D_\theta}\zeta_i(t)\,, \tag{7}$$

where $\langle \zeta_i(t) \rangle = 0$ and $\langle \zeta_i(t)\zeta_j(t') \rangle = \delta_{i,j}\delta(t-t)$. Compute the mean square displacement of the particles for various D_θ values, and compare the results with the theory.

4

Simulate a system of N interacting self-propelled particles moving on a two-dimensional space with periodic boundary conditions. The particle-particle interaction is given by a polar alignment mechanism. The equation of motion of the i-th particle is given by :

$$\dot{\mathbf{x}}_i = v_0(\cos(\theta_i), \sin(\theta_i)) \tag{8}$$
$$\dot{\theta}_i = \frac{\gamma}{n_i(t)} \sum_{|\mathbf{x}_i - \mathbf{x}_j| < R} \sin(\theta_j - \theta_i) + \sqrt{2D_\theta}\zeta_i(t)\,, \tag{9}$$

where $n_i(t)$ is the number of particles that are located at a distance smaller or equal to R from $\mathbf{x}_i$, $\langle \zeta_i(t) \rangle = 0$ and $\langle \zeta_i(t)\zeta_j(t') \rangle = \delta_{i,j}\delta(t-t)$. Compute the polar order parameter as function of D_θ and estimate the critical value of D_θ for $\gamma = 1$. Recall that the polar order parameter is defined by $\phi = |\frac{1}{N}\sum_{i=1}^{N} \exp(i\theta_i(t))|$.