M2 - Physics of Complex Systems - 2020-2021

Non-equilibrium dynamics

Homework N°1.

I- Equipartition theorem and Itō calculus

We consider a particle of mass m, position $x(t)$ and momentum $p(t)$ in a quadratic potential $V(x) = \frac{1}{2}\omega x^2$. The Boltzmann constant is $\beta = (kT)^{-1}$ and the particle mobility $\mu = \frac{1}{\gamma}$.

A) Write down the Langevin dynamics of $x(t)$ and $p(t)$. Show that in the large damping limit ($\gamma \to \infty$) it reduces to

$$\dot{x}(t) = -\frac{\omega}{\gamma}x(t) + \sqrt{\frac{2kT}{\gamma}}\eta(t) \tag{1}$$

where $\eta(t)$ is a zero-mean unit-variance Gaussian white noise. Show that its solution is

$$x(t) = x(0)\mathrm{e}^{-\frac{\omega}{\gamma}t} + \sqrt{\frac{2kT}{\gamma}}\int_0^t \mathrm{e}^{-\frac{\omega}{\gamma}(t-s)}\eta(s)\mathrm{d}s \tag{2}$$

Compute $\langle x(t)\rangle$ and $\langle x(t)^2\rangle$ and show that, in steady-state,

$$\langle V(x)\rangle = \frac{kT}{2}. \tag{3}$$

B) Using Itō formula, construct the dynamics of $x^2(t)$ starting from Eq. (1). What is the first order differential equation satisfied by $\langle x^2(t)\rangle$? Solve it for an initial distribution $P[x(t=0)] = \delta(x)$ and deduce Eq. (3) in steady-state.

C) Let us now consider N Brownian particles of positions x_i, interacting via the potential

$$V(x_1, \dots, x_N) = \frac{1}{2}\sum_{i,j=1}^{N} x_i \Omega_{ij} x_j$$

where Ω is a symmetric positive-definite matrix and the particles experience N independent noises $\eta_i(t)$. What is the overdamped Langevin dynamics of each oscillator? Using Itō formula, show that

$$\frac{1}{2}\frac{d}{dt}(\vec{x}\cdot\vec{x}) = -\mu\vec{x}\cdot\Omega\vec{x} + \sqrt{2\mu kT}\vec{x}\cdot\vec{\eta} + \mu NkT \tag{4}$$

Is equipartition satisfied in steady-state?

D) We now consider the underdamped dynamics: $m\dot{q} = p$ and $\dot{p} = -\gamma p/m - V'(q) + \sqrt{2\gamma kT}\eta(t)$. Construct the evolution equations of $\langle q^2(t)\rangle$, $\langle V\big(q(t)\big)\rangle$, $\langle q(t)p(t)\rangle$ and $\langle p^2(t)\rangle$ and show that in steady-state

$$\langle qp\rangle = \langle pV'(q)\rangle = 0 \quad ; \quad \left\langle\frac{p^2}{m}\right\rangle = \langle qV'(q)\rangle = kT \tag{5}$$

II- The Dean-Kawasaki Equation

Let us consider N interacting particles

$$\dot{x}_i = -\sum_j V'(x_i - x_j) + \eta_i; \qquad \langle \eta_i \rangle = 0; \qquad \langle \eta_i(t)\eta_j(t') \rangle = 2kT\delta_{i,j}\delta(t-t') \tag{6}$$

where $V(u)$ is the interaction potential.

A) Show that

$$\rho(x,t) = \sum_i \delta\Big(x - x_i(t)\Big)$$

is a distribution which measures a *local* density of particles.

B) We consider a differentiable function $f(x)$ and define

$$F(t) = \sum_i f(x_i(t)) \tag{7}$$

Using the definition of $\rho(x,t)$, show that

$$\dot{F}(t) = \int dx f(x)\dot{\rho}(x,t)$$

C) Using Itō formula on equation (7), show that $\dot{F}(t)$ can be alternatively written as

$$\dot{F}(t) = \int dx f(x)\partial_x[kT\partial_x\rho(x,t) + \int dy V'(x-y)\rho(x)\rho(y) - \sum_i \eta_i\delta(x - x_i(t))] \tag{8}$$

Hint: $g(x_i)$ can always be written as $\int g(x)\delta(x - x_i)$. Show that the density $\rho(x,t)$ evolves as

$$\dot{\rho}(x,t) = \partial_x[kT\partial_x\rho(x,t) + \int \mathrm{d}y V'(x-y)\rho(x,t)\rho(y,t) + \xi(x,t)] \tag{9}$$

where $\xi(x,t)$ is a random variable. Give its expression in terms of x, η_i and $x_i(t)$.

D) Show that

$$\langle \xi(x,t) \rangle = 0 \quad \text{et} \quad \langle \xi(x,t)\xi(x',t') \rangle = \delta(t-t')\delta(x-x')\rho(x,t)2kT \tag{10}$$

where $\langle \dots \rangle$ are averages over the noises $\eta_i(t)$ for given density profiles $\rho(x,t)$ and $\rho(x',t')$.

E) Show that the dynamics (9) can be written as

$$\dot{\rho}(x,t) = \partial_x[\rho(x,t)\partial_x \frac{\delta\mathcal{F}[\rho]}{\delta\rho(x,t)} + \xi(x,t)] \tag{11}$$

Give the expression of the functional $\mathcal{F}[\rho]$ and its interpretation.