8.08/8.S308 - Problem Set 2 - IAP 2025

Due before January 16, 23:59

Anything marked as "graduate" count as bonus problems for undergraduate students.

1- 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 $\mu = \frac{1}{\gamma}$.

1.1) Write down the underdamped 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 the steady state,

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

1.2) Using Itō formula, construct the time-evolution equation 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 the steady state.

1.3) 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 the steady state?

1.4) 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 the steady state,

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

2- Geometrical Brownian Motion

We consider the celebrated Black–Scholes model, which describes the evolution of the value $y(t)$ of an investment using the Itō-Langevin equation:

$$\dot{y}(t) = f\, y(t) + \sqrt{2D}\, y(t)\, \eta(t)\ , \tag{6}$$

where f and D are real numbers and $\eta(t)$ is a Gaussian white noise of zero mean and unit variance $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$.

2.1) Determine the equations of evolution of $\langle y(t)\rangle$ and $\langle y(t)^2\rangle$.

2.2) Compute the mean and the variance of y at time t knowing that $y(t=0) = y_0 > 0$.

2.3) If f is negative, show that the value of $y(t)$ is going down on average. Depending on the value of D, do you think that $\langle y(t)\rangle$ is a reliable prediction for the value of $y(t)$ at large times?

2.4) We now consider the stochastic process $x(t) = h(y(t))$ where h is a strictly increasing smooth function, defined for $y > 0$. Compute $\frac{d}{dt}x(t)$ in terms, among other things, of $y(t)$ and $\eta(t)$.

2.5) The variance of the noise term in (6) depends on $y(t)$, this is called a multiplicative noise. What is the condition on h under which the statistics of the noise term in the Langevin equation for $x(t)$ does *not* depend on x (i.e. the noise is additive)?

2.6) We now consider the case $y(t) = \exp[x(t)]$. Show that, for this choice, the dynamics of x read:

$$\dot{x} = f - D + \sqrt{2D}\eta(t) \tag{7}$$

2.7) We now consider the case $D = f$. Give without derivation the Fokker-Planck equation describing the evolution of $P_x(x,t)$, the probability density that the random variable $x(t)$ takes value x at time t?

2.8) We define the Fourier transform of P_x as

$$\hat{P}_x(q,t) = \int_{-\infty}^{\infty} dx P_x(x,t) e^{-iqx} \tag{8}$$

If the initial condition is given by $y(t=0) = y_0$, what are the values of $P_x(x,0)$ and $\hat{P}_x(q,0)$?

2.9) Show that $\partial_t \hat{P}_x(q,t) = -Dq^2 \hat{P}_x(q,t)$.

2.10) Solve this equation and inverse the Fourier transform to get

$$P_x(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left[-\frac{(x - \ln(y_0))^2}{4Dt}\right] \tag{9}$$

2.11) We now want to infer $P_y(y,t)$, the probability density that the random variable $y(t)$ solution of (6) (with $D = f$) takes value y at time t, knowing that it was at y_0 at time zero. To do so, we consider first the case of two general random variables x and y such that $x = h(y)$ with h an increasing function. Again, we note $P_x(x)$ and $P_y(y)$ the probability densities associated to the two variables. Explain the physical meanings of

$$F_x(\bar{x}) = \int_{-\infty}^{\bar{x}} dx P_x(x); \qquad \text{and} \qquad F_y(\bar{y}) = \int_{-\infty}^{\bar{y}} dy P_y(y) \tag{10}$$

2.12) For each $\bar{y}$, for what value $\bar{x}(\bar{y})$ do we have $F_x(\bar{x}(\bar{y})) = F_y(\bar{y})$? Taking the derivative of this equality with respect to a wisely chosen variable, show that

$$P_y(\bar{y}) = P_x(h(\bar{y}))h'(\bar{y}) \tag{11}$$

2.13) Conclude that the distribution of the solution of (6) (with $D = f$) knowing that $y(t = 0) = y_0$ is

$$P_y(y,t) = \frac{1}{y\sqrt{4\pi Dt}} \exp\left[-\frac{\Big(\ln(y) - \ln(y_0)\Big)^2}{4Dt}\right] . \tag{12}$$

3. *Graduate:* The Dean-Kawasaki Equation

Let us consider N interacting particles

$$\dot{x}_i = -\sum_j V'(x_i - x_j) + \eta_i; \qquad \langle \eta_i \rangle = 0; \qquad \langle \eta_i(t)\eta_j(t') \rangle = 2kT\delta_{i,j}\delta(t-t') \tag{13}$$

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

3.1) Show that

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

is a distribution which measures the *local* (number) density of particles.

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

$$F(t) = \sum_i f(x_i(t)) \tag{14}$$

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

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

3.3) Using Itō formula on equation (14), show that $\dot{F}(t)$ can be alternatively written as

$$\dot{F}(t) = \int dx f(x)\partial_x[kT\partial_x\rho(x,t) + \int dy V'(x-y)\rho(x)\rho(y) - \sum_i \eta_i\delta(x - x_i(t))] \tag{15}$$

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

$$\dot{\rho}(x,t) = \partial_x[kT\partial_x\rho(x,t) + \int \mathrm{d}y V'(x-y)\rho(x,t)\rho(y,t) + \xi(x,t)] \tag{16}$$

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

3.4) Show that

$$\langle \xi(x,t) \rangle = 0 \quad \text{et} \quad \langle \xi(x,t)\xi(x',t') \rangle = \delta(t-t')\delta(x-x')\rho(x,t)2kT \tag{17}$$

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

3.5) Show that the dynamics (16) can be written as

$$\dot{\rho}(x,t) = \partial_x\left[\rho(x,t)\partial_x\frac{\delta\mathcal{F}[\rho]}{\delta\rho(x,t)} + \xi(x,t)\right] \tag{18}$$

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