8.08/8.S308 - Problem Set 3 - IAP 2025

Due before January 22, 23:59

Anything marked as "graduate" counts as bonus problem for undergraduate students.

1- Backward Fokker-Planck Equation

The dynamics of a colloidal particle can be described, at the trajectory level, by a stochastic equation:

$$\dot{x} = f(x) + \sqrt{2D(x)}\eta(t); \qquad \text{with} \qquad \langle \eta(t) \rangle = 0; \qquad \langle \eta(t)\eta(t') \rangle = \delta(t-t'); \tag{1}$$

and, at the level of probability distribution, through a Fokker-Planck equation

$$\frac{\partial P(x,t|x_0,t_0)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}D(x) - f(x)\right] P(x,t|x_0,t_0) \tag{2}$$

where $P(x,t|x_0,t_0)$ is the probability to find the colloid at x at time t knowing that it was at x_0 at time t_0. This equation is called the "Forward Fokker-Planck equation" because, once the system has been at x_0 at time t_0, it describes what happens in the future (Fig. 1, left).

Conversely, $P(x,t|x_0,t_0)$ can be seen as a function of the variables x_0 and t_0: what is the probability of reaching x at time t if leaving x_0 at t_0. One can thus study how $P(x,t|x_0,t_0)$ evolves *with* t_0 (cf Fig. 1, right). This is the purpose of the Backward Fokker-Planck equation, which we construct in this exercise.

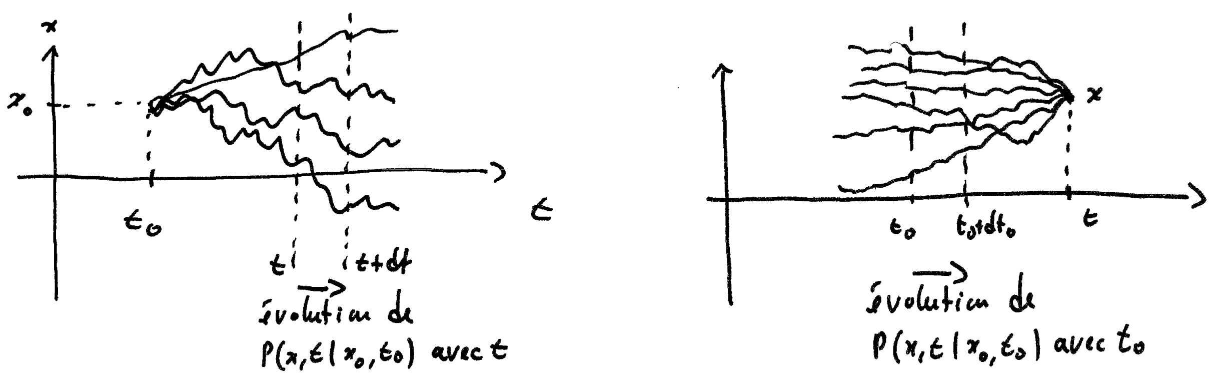

Figure 1: *$P(x,t|x_0,t_0)$ can be seen either as a function of x,t, for fixed values of x_0 and t_0—this is the perspective of the forward Fokker-Planck equation (left)—or as a function of x_0 and t_0, for fixed values of x and t—this is the point of view of the backward Fokker-Planck equation (right).*

1.1) Consider a particle evolving with equation (1). The probability to find it at x_0, x' and x at the successive times $t_0 < t' < t$, $P(x,t;x',t';x_0,t_0)$, satisfies

$$P(x,t;x',t';x_0,t_0) = P(x,t|x',t')P(x',t'|x_0,t_0)P(x_0,t_0) \tag{3}$$

where $P(x_0,t_0)$ is the probability that the particle was at x_0 at t_0. Explain intuitively the content of equation (3). On which property of the dynamics (1) does equation (3) rely?

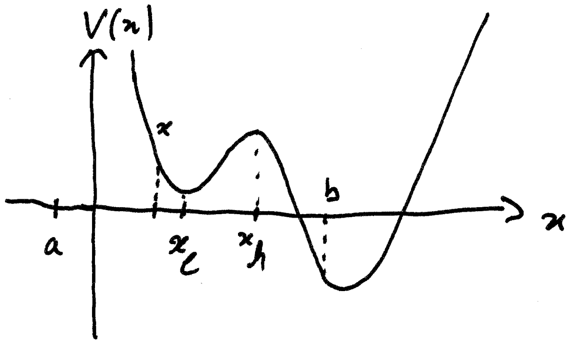

Figure 2: Energy landscape leading to the existence of a metastable state around x_ℓ, separated from the main energy well by an energy barrier. We want to compute the mean first-passage time from x to b.

1.2) For three random variables a,b,c, one has $P(a,c) = \int \mathrm{d}b P(a,b,c)$. Apply this formula to $P(x,t;x',t';x_0,t_0)$ to show that $P(x,t|x_0,t_0)$ is solution of the Chapman-Kolmogorov equation:

$$\forall t' \in]t, t_0[, \qquad P(x,t|x_0,t_0) = \int \mathrm{d}x' P(x,t|x',t')P(x',t'|x_0,t_0) \tag{4}$$

What is the physical meaning of equation (4)?

1.3) Take the derivative of equation (4) with respect to t' and show that $P(x,t|x_0,t_0)$ is solution of the Backward Fokker-Planck equation:

$$\frac{\partial P(x,t|x_0,t_0)}{\partial t_0} = -\left[D(x_0)\frac{\partial}{\partial x_0} + f(x_0)\right]\frac{\partial}{\partial x_0}P(x,t|x_0,t_0) \tag{5}$$

Hint: Remember that $\lim_{t'\to t_0} P(x',t'|x_0,t_0) = \delta(x'-x_0)$

1.4) For a stochastic process which does not explicitly depend on time (a.k.a. 'homogeneous in time'), one has $P(x,t|x_0,t_0) = P(x,t+\tau|x_0,t_0+\tau)$. Show this to imply that

$$\partial_t P(x,t|x_0,t_0) = -\partial_\tau P(x,0|x_0,\tau = t_0 - t) \tag{6}$$

Using the Backward Fokker-Planck, applied to $P(x,0|x_0,t_0-t)$, show that

$$\frac{\partial P(x,t|x_0,t_0)}{\partial t} = \left[D(x_0)\frac{\partial}{\partial x_0} + f(x_0)\right]\frac{\partial}{\partial x_0}P(x,t|x_0,t_0) \tag{7}$$

2- The Kramers Problem

We study the time it takes for a particle evolving with the Langevin dynamics

$$\dot{x} = -V'(x) + \sqrt{2kT}\eta(t) \qquad \text{where} \qquad \langle\eta(t)\rangle = 0; \qquad \langle\eta(t)\eta(t')\rangle = \delta(t-t') \tag{8}$$

to cross an energy barrier of height ΔE (Fig 2). More precisely, we would like to compute the mean first-passage time to reach b for a particle that was at x at $t=0$.

2.1) We use absorbing boundary conditions at a and b, i.e. a particle reaching a or b is removed from the system. What does the function

$$G(x,t) = \int_a^b \mathrm{d}x' P(x',t|x,0) \tag{9}$$

measure ?

2.2) $G(x,t+dt)$ and $G(x,t)$ are not necessarily equal. Why? How is their difference connected to $Q(x,t)dt$, the probability that a particle leaves $[a,b]$ for the first time between t and $t+dt$? Show that

$$Q(x,t) = -\partial_t G(x,t) \tag{10}$$

What is the mathematical definition of $\bar{Q}(x)$, the mean time it takes for the particles to exit $[a,b]$? Show that

$$\bar{Q}(x) = \int_0^\infty G(x,t)dt \tag{11}$$

(We admit without proof that $\lim_{t\to\infty} tG(x,t) = 0$.)

2.3) Using the Backward Fokker-Planck equation, show that $G(x,t)$ is a solution of

$$\partial_t G(x,t) = kT\frac{\partial^2}{\partial x^2}G(x,t) - V'(x)\frac{\partial}{\partial x}G(x,t) \tag{12}$$

Then, show that $\bar{Q}(x)$ is a solution of the ordinary differential equation

$$kT\bar{Q}''(x) - V'(x)\bar{Q}'(x) = -1 \tag{13}$$

2.4) We now take $a = -\infty$, so that particles only exit $[a,b]$ at $x = b$. Show that the mean first-passage time until b is given by:

$$\bar{Q}(x) = \frac{1}{kT}\int_x^b \mathrm{d}s\, e^{\beta V(s)} \int_{-\infty}^s \mathrm{d}u\, e^{-\beta V(u)} \tag{14}$$

(To do so, simply check that this expression is a solution of (13) with the proper boundary condition as $x \to b$.)

2.5) *Graduate.* We now turn to the low temperature limit. For x and b as in Fig 2, show that the integral over s is dominated by the vicinity of x_h when $T \to 0$ and that the integral over u is dominated by the vicinity of x_ℓ. Using a Taylor expansion of the potential around these points, prove the validity of the Arrhenius law:

$$\bar{Q}(x) \underset{T\to 0}{\simeq} \frac{2\pi}{\sqrt{|V''(x_h)V''(x_\ell)|}} e^{\beta[V(x_h)-V(x_\ell)]} \tag{15}$$

2.6) *Graduate.* Does this result depend on x? on b? What is the typical time-scale for this system to reach its steady-state?

Graduate: 3- Non-equilibrium dynamics with 2 degrees of freedom

Let us consider the Itō-Langevin dynamics

$$\gamma_1\dot{x}_1 = f_1(x_1,x_2) + \sqrt{2\gamma_1 T_1}\eta_1; \qquad \gamma_2\dot{x}_2 = f_2(x_1,x_2) + \sqrt{2\gamma_2 T_2}\eta_2; \tag{16}$$

where μ_i and T_i are positive constants, and $\eta_1(t)$ and $\eta_2(t)$ are two independent Gaussian White Noises of statistics $\langle\eta_i\rangle = 0$ and $\langle\eta_i(t)\eta_j(t')\rangle = \delta_{i,j}\delta(t-t')$. The force field $\vec{f} = (f_1, f_2)$ is smooth.

3.1) We consider $P(x_1^0, x_2^0, t)$ the density of probability to observe the stochastic processes $x_1(t)$ and $x_2(t)$, solutions of (16), at positions x_1^0 and x_2^0 at time t. Show that

$$P(x_1^0, x_2^0, t) = \langle \delta(x_1(t) - x_1^0)\delta(x_2(t) - x_2^0) \rangle_{x_1, x_2} \tag{17}$$

where the average is computed over the realisations of the stochastic processes $x_1(t)$ and $x_2(t)$.

3.2) Taking the derivative of (17) with respect to time, and using Itō calculus where appropriate, show that $P(x_1^0, x_2^0, t)$ is solution of the Fokker-Planck equation

$$\partial_t P(x_1^0, x_2^0, t) = \frac{\partial}{\partial x_1^0}\left[\frac{\partial}{\partial x_1^0}\mu_1 T_1 - \mu_1 f_1\right] P(x_1^0, x_2^0, t) + \frac{\partial}{\partial x_2^0}\left[\frac{\partial}{\partial x_2^0}\mu_2 T_2 - \mu_2 f_2\right] P(x_1^0, x_2^0, t) \tag{18}$$

where we have introduced the mobilities $\mu_i = \frac{1}{\gamma_i}$. You can neglect all boundary terms when doing integration by parts.

3.3) We drop the superscript x_i^0 from now on. Show that the Fokker-Planck equation (18) can be put under the form of a conservation equation $\partial_t P(x_1, x_2, t) = -\nabla \cdot \vec{J}$ and give the expression of $\vec{J} = (J_1, J_2)$.

3.4) We consider $f_i = -\partial_{x_i} U(x_1, x_2)$, where U is a smooth potential which depends explicitly on x_1 and x_2. Under which conditions does the current $\vec{J}$ vanish in the steady state? What is the expression of $P(x_1, x_2)$ in such steady states?

3.5) We now consider $\mu_i = 1$, $T_i = T$ and $\vec{f} = -\nabla U + \vec{g}$, where $\vec{g}$ is *not* the gradient of a potential. Show that if $\vec{g} \cdot \nabla U = 0$ and $\nabla \cdot \vec{g} = 0$, then $P = \exp[-U/T]/Z$ is an acceptable steady-state (if U is a confining potential and Z a normalization constant). Does the current vanish in steady-state?