Chapter 4

The Fokker-Planck Equation

4.1 From Langevin to Fokker-Planck

4.1.1 A direct application of Itō's lemma

We begin the discussion with a simple goal in mind. Given an Itō-discretized Langevin equation $\dot{x} \overset{0}{==} f + g\eta$, how can we find an equation for the probability density $p(X,t)$ such that $p(X,t)\mathrm{d}X = \mathrm{Prob}\{X \le x(t) \le X + \mathrm{d}X\}$. The idea is to remark that

$$p(X,t) = \langle \delta(X - x(t)) \rangle \tag{4.1}$$

because indeed, for any physical quantity $A(x(t))$, its average is given by

$$\langle A \rangle(t) = \int \mathrm{d}X A(X) p(X,t) = \langle \int \mathrm{d}X A(X) \delta(X - x(t)) \rangle \tag{4.2}$$

We directly apply Itō's lemma, namely

$$\dot{u} = U'(f + g\eta) + \frac{1}{2} g^2 U'' \tag{4.3}$$

to $u(t) = U(x(t)) = \delta(X - x(t))$, and then we take the average:

$$\langle \dot{u} \rangle = \langle U' f + \frac{1}{2} g^2 U'' \rangle \tag{4.4}$$

This directly tells us that

$$\partial_t p = \langle f \frac{\partial}{\partial x} \delta(X - x) + \frac{1}{2} g^2 \frac{\partial^2}{\partial x^2} \delta(X - x) \rangle \tag{4.5}$$

so that, using that $\frac{\partial}{\partial x}\delta(X-x) = -\frac{\partial}{\partial X}\delta(X-x)$, we arrive at

$$\partial_t p = -\partial_X (fp) + \frac{1}{2} \partial_X^2 (g^2 p) \tag{4.6}$$

A direct application is thus that for a Langevin equation in the Markov approximation and the overdamped limit,

$$\dot{\mathbf{r}} = \mu\mathbf{F} + \sqrt{2\mu T}\boldsymbol{\eta},\ \mu = \gamma^{-1} \tag{4.7}$$

where $\mathbf{F} = -\partial_{\mathbf{r}} V + \mathbf{f}$ is an external force field comprising a conservative part and a nonconservative one, we have

$$\partial_t p = \mu\partial_{\mathbf{r}} \cdot ([\partial_{\mathbf{r}} V - \mathbf{f}]p) + \mu T \partial_{\mathbf{r}} p \tag{4.8}$$

Of course, one can check that when $\mathbf{f} = \mathbf{0}$ we have that $p_{\text{eq}}(\mathbf{r}) = \text{e}^{-\beta V(\mathbf{r})}/Z$ is a stationary solution of Eq. (4.8).

4.1.2 Higher-dimensional Fokker-Planck equation

Suppose that we start from a higher-dimensional process

$$\dot{x}_\mu \overset{0}{=} f_\mu + g_{\mu i}\eta_i \tag{4.9}$$

where the noises verify $\langle \eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t-t')$. While the dimensionality index μ runs from 1 to d, the noise index i doesn't have to run up to d. In other words the matrix $g_{\mu i}$ doesn't have to be square, but it cannot have more columns than lines. Itō's lemma for a function $u(t) = U(x_1(t),\dots,x_d(t))$ takes a somewhat more complex form:

$$\dot{u} = \partial_\mu U \dot{x}_\mu + \frac{1}{2} g_{\mu j} g_{\nu j} \partial_\mu \partial_\nu U \tag{4.10}$$

One way to verify this formula is to *a posteriori* determine $\frac{\langle \Delta u\rangle}{\Delta t}$ in the $\Delta t \to 0$ limit directly from the equation on x_μ. The reason why we may need such an extension of Itō's lemma is that we'd like to be able to find the Fokker-Planck equation for more complex processes than an overdamped Langevin particle. But actually, the simplest situation where this extension is need is for the underdamped particle:

$$\dot{\mathbf{r}} = \mathbf{v},\ m\dot{\mathbf{v}} = -\gamma\mathbf{v} - \partial_{\mathbf{r}} V + \sqrt{2\gamma T}\boldsymbol{\eta} \tag{4.11}$$

then the joint variable $\mathbf{X} = \begin{pmatrix} \mathbf{r} \\ \mathbf{v} \end{pmatrix}$ is Markovian and its evolution reads

$$\dot{X}_\mu = F_\mu(\mathbf{r},\mathbf{v}) + g_{\mu j}(\mathbf{r},\mathbf{v})\eta_j \tag{4.12}$$

with $\mathbf{F} = \begin{pmatrix} \mathbf{v} \\ -\partial_{\mathbf{r}} V/m - \gamma\mathbf{v}/m \end{pmatrix}$ and the matrix $g_{\mu j}$ given by (for $d = 3$)

$$g_{\mu j} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \sqrt{2\gamma T}/m & 0 & 0 \\ 0 & \sqrt{2\gamma T}/m & 0 \\ 0 & 0 & \sqrt{2\gamma T}/m \end{pmatrix} \tag{4.13}$$

The index μ runs from 1 to $2d$ (where d is the position space dimension), while the noise index $i = 1$ runs only from 1 to d. We now apply Itō's lemma to $u(t) = U(\mathbf{x}(t)) = \delta(\mathbf{x}–\mathbf{r}(t))\delta(\mathbf{w}–\mathbf{v}(t))$ and we take the average. Denoting by

$$p(\mathbf{x}, \mathbf{w}, t) = \langle u(t)\rangle = \langle \delta(\mathbf{x} - \mathbf{r}(t))\delta(\mathbf{w} - \mathbf{v}(t))\rangle \tag{4.14}$$

we readily arrive at the Fokker-Planck equation

$$\partial_t p = \frac{1}{m}\partial_{\mathbf{w}}((\gamma\mathbf{w} + \partial_{\mathbf{r}} V)p) - \mathbf{w}\cdot\partial_{\mathbf{r}} p + \frac{T}{m}\partial^2_{\mathbf{w}} p \tag{4.15}$$

Needless to say, $p_{\text{eq}}(\mathbf{x}, \mathbf{w}) = \mathrm{e}^{-\frac{1}{T}\left(m\mathbf{w}/2+V(\mathbf{x})\right)}$ is a stationary solution of that Fokker-Planck equation.

4.1.3 Infinitesimal moments, and more complex averages

Once a Fokker-Planck equation for a process $x(t)$ is known, say of the form

$$\partial_t p = -\partial_\mu(a^{(1)}_\mu p) + \frac{1}{2}\partial_\mu\partial_\nu(a^{(2)}_{\mu\nu} p) = -\mathbb{H}p \tag{4.16}$$

then we can ask about the statistics of the infinitesimal jump $\Delta x_\mu = x_\mu(t_0 + \Delta t) - x_\mu(t_0)$ starting from a fixed value $x(t_0) = x_0$ at $t = t_0$, and averaging over the realizations of the noise during the $[t_0, t_0 + \Delta t]$ interval. Here the notation $\mathbb{H}$ refers to the differential operator acting on p. Let us denote by $p(x, t|x_0, t_0)$ the solution of the Fokker-Planck equation with the initial condition $p(x, t_0|x_0, t_0) = \delta(x - x_0)$. Then, for instance,

$$\langle\Delta x_\mu\rangle = \int \mathrm{d}x' x'_\mu p(x_0 + x', t_0 + \Delta t|x_0, t_0) \tag{4.17}$$

But for Δt very small, we can write

$$p(x_0 + x', t_0 + \Delta t|x_0, t_0) = p(x_0 + x', t_0|x_0, t_0) + \Delta t\partial_t p(x_0 + x', t_0|x_0, t_0) + O(\Delta t^2) \tag{4.18}$$

so that, using that $p(x_0 + x', t_0|x_0, t_0) = \delta(x')$, we immediately find that

$$\langle\Delta x_\mu\rangle = \Delta t \int \mathrm{d}x' x'_\mu \underbrace{\partial_t p(x_0 + x'|t_0|x_0, t_0)}_{-\partial_\nu(a^{(1)}_\nu(x_0+x')p+\frac{1}{2}\partial_\mu\partial_\nu(a^{(2)}_{\mu\nu}(x_0+x')p} + O(\Delta t^2) \tag{4.19}$$

With a couple of integration by parts we then arrive at

$$\langle\Delta x_\mu\rangle = \Delta t a^{(1)}_\mu(x_0) + O(\Delta t^2) \tag{4.20}$$

and a similar reasoning leads to

$$\langle\Delta x_\mu\Delta x_\nu\rangle = \Delta t a^{(2)}_{\mu\nu}(x_0) + O(\Delta t^2) \tag{4.21}$$

while any higher moment of Δx is negligible with respect to Δt. This gives us a recipe to work a Langevin equation backwards from a Fokker-Planck one:

$$\dot{x}_\mu \overset{0}{=} a_\mu^{(1)} + \xi_\mu,\ \langle \xi_\mu(t)\xi_\nu(t')\rangle = a_{\mu\nu}^{(2)}(x)\delta(t-t') \tag{4.22}$$

where the Itō-discretization was used.

Of course, the average of a given observable $A(t) = A(x(t))$ that depends on the random variable x is given by

$$\langle A\rangle(t) = \int \mathrm{d}x A(x)p(x,t) \tag{4.23}$$

and thus the average is a solution of

$$\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = \int \mathrm{d}x A(x)(-\partial_\mu(a_\mu^{(1)}p) + \frac{1}{2}\partial_\mu\partial_\nu(a_{\mu\nu}^{(2)}p)) \tag{4.24}$$

again, using integration by parts, one see that

$$\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = \int \mathrm{d}x \left[a_\mu^{(1)}\partial_\mu A(x) + \frac{1}{2}a_{\mu\nu}^{(2)}\partial_\mu\partial_\nu A)\right] p = -\int \mathrm{d}x(\mathbb{H}^\dagger A)p \tag{4.25}$$

Let $q(x) = 1$, then, introducing the notation $\langle f|g\rangle = \int \mathrm{d}x f(x)g(x)$ we see that

$$\langle A\rangle = \langle q|\hat{A}p\rangle,\ \hat{A} = A(x) \tag{4.26}$$

and

$$\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = -\langle q|\mathbb{H}^\dagger\hat{A}p\rangle = \langle q|\hat{A}\mathbb{H}p\rangle = \langle q|[\mathbb{H},\hat{A}]p\rangle \tag{4.27}$$

where we have used that $\langle q|\mathbb{H}\phi\rangle = 0$ for any ϕ. Indeed, this is obvious when we make things more explicit:

$$\langle q|\mathbb{H}\phi\rangle = \int \mathrm{d}x \left(-\partial_\mu(a_\mu^{(1)}\phi) + \frac{1}{2}\partial_\mu\partial_\nu(a_{\mu\nu}^{(2)}\phi)\right) = 0 \tag{4.28}$$

after on or two integration by parts. The vector $\langle q|$ is an eigenstate of $\mathbb{H}^\dagger$ with eigenvalue 0, so that at least we know that 0 is an eigenvalue and there must be a corresponding eigenstate for $\mathbb{H}$: this eigenvector is the steady-state probability.

Suppose now that we want to determine, for $t > 0$, the correlation function $\langle B(t)A(0)\rangle$, where both A and B are x-dependent random variables. The brackets refer to an average over the initial state (whenever this was, whether at $t = 0$ or at some earlier time) and over the noise realization up until time t. Let us assume that at time $t = 0$ the value of $x(0) = x_0$ is fixed. Then $A(0) = A(x_0)$. For that initial condition, the value of x at t is $x(t)$, and $B(t) = B(x(t))$, so that the quantity $\langle B(t)\rangle|_{\text{at fixed } x(0)=x_0} A(0)$ is the product of $B(t)$ by $A(0)$, averaged over all trajectories, at fixed initial state. One can in addition average over the initial state at $t = 0$ and then

$$\int \mathrm{d}x_0 p(x_0, t=0)\ \langle B(t)\rangle|_{\text{at fixed } x(0)=x_0} A(0) = \langle B(t)A(0)\rangle \tag{4.29}$$

The quantity $J_\mu(x,t) = a_\mu^{(1)}p(x,t) - \frac{1}{2}\partial_\nu(a_{\mu\nu}^{(2)}p(x,t))$ is the probability current. For an overdamped Langevin equation $\gamma\dot{\mathbf{r}} = \mathbf{F} + \sqrt{2\gamma T}\boldsymbol{\eta}$, its first contribution $\frac{1}{\gamma}\mathbf{F}p$ is the deterministic drift, while the $-D\partial_{\mathbf{x}}p$ term (wiht $D = T/\gamma$) expresses Fick's law (in the absence of external drift, p is the solution of a diffusion equation).

4.1.4 Spectrum and relaxation

When we write $\partial_t p = -\mathbb{H}p$, the operator $\mathbb{H}$ must have certain properties. We have already seen that it conserves probability ($q(x) = 1$ is an eigenvector of $\mathbb{H}^\dagger$ with eigenvalue 0), but it must also conserve the positivity of p. If we start from a normalized an positive function $p(x, 0)$, how can we be sure that $p(x, t)$ remains positive at all times, just by seeing the equation (of course, we know this must be true)? How can we be sure that there will exist a steady-state? Will it be unique? All these are interesting and fundamental questions, that we will address later, by the example.

In the case of an overdamped Langevin equation $\dot{\mathbf{r}} = \mathbf{F} + \sqrt{2T}\boldsymbol{\eta}$, where the force field $\mathbf{F} = -\boldsymbol{\nabla}\mathbf{V}$ is necessarily conservative, we can determine the operator $\mathrm{e}^{\beta V/2}\mathbb{H}\mathrm{e}^{-\beta V/2}$ which, for $-\mathbb{H}\bullet = T\boldsymbol{\nabla}^2\bullet - \boldsymbol{\nabla}\cdot(\mathbf{F}\bullet)$ becomes

$$\mathrm{e}^{\beta V/2}\mathbb{H}\mathrm{e}^{-\beta V/2} = \mathbb{H}_s \tag{4.30}$$

where $\mathbb{H}_s\bullet = -T\boldsymbol{\nabla}^2\bullet + \left[\frac{\beta}{4}(\boldsymbol{\nabla}V)^2 - \frac{1}{2}\boldsymbol{\nabla}^2 V\right]$ which is manifestly symmetric (and thus Hermitian because it is real). But it is furthermore easy to see that the spectrum of $\mathbb{H}_s$ is positive semi-definite, since

$$\mathbb{H}_s = T\left[\boldsymbol{\nabla} + \frac{\beta}{2}\boldsymbol{\nabla}V\right]^\dagger\left[\boldsymbol{\nabla} + \frac{\beta}{2}\boldsymbol{\nabla}V\right] \tag{4.31}$$

When $\mathbf{F}$ is arbitrary, it takes a bit more work. Then we denote by $U(\mathbf{r}) = -\frac{1}{\beta}\ln p_{\rm ss}(\mathbf{r})$ a function built from the steady-state distribution $p_{\rm ss}$. By construction, U verifies $-\boldsymbol{\nabla}\cdot\mathbf{F} + \beta\boldsymbol{\nabla}U\cdot(\mathbf{F} + \boldsymbol{\nabla}U) - \boldsymbol{\nabla}^2 U = 0$. Then we construct the combination $\mathrm{e}^{\beta U/2}\mathbb{H}\mathrm{e}^{-\beta U/2}$ which we split as follows:

$$\mathrm{e}^{\beta U/2}\mathbb{H}\mathrm{e}^{-\beta U/2} = \mathbb{H}_s + \mathbb{H}_a \tag{4.32}$$

where

$$\mathbb{H}_s\bullet = T\left[\boldsymbol{\nabla} + \frac{\beta}{2}\boldsymbol{\nabla}U\right]^\dagger\left[\boldsymbol{\nabla} + \frac{\beta}{2}\boldsymbol{\nabla}U\right]\bullet \tag{4.33}$$

is manifestly Hermitian and semi-positive-definite. The other contribution $\mathbb{H}_a$ reads

$$\mathbb{H}_a\bullet = (\mathbf{F} + \boldsymbol{\nabla}U)(\boldsymbol{\nabla} + \beta\boldsymbol{\nabla}U/2)\bullet \tag{4.34}$$

and using the equation connecting U to $\mathbf{F}$ one sees that $\mathbb{H}_a^\dagger = -\mathbb{H}_a$. It turns out that when the spectrum of some symmetric operator $\mathbb{H}_s$ is positive semi-definite, then for each of its eigenvalue λ_s we can prove that the eigenvalue λ of $\mathbb{H}_s + \mathbb{H}_a$ verifies $\Re(\lambda) > \lambda_s$ when $\mathbb{H}_a$ is antisymmetric.

In practice, if we are able to diagonalize $\mathbb{H}$, then things will become simpler for us: assume we have found the λ's and r_λ's such that $\mathbb{H}|r_\lambda\rangle = \lambda|\phi\rangle$. Then we know that $p(x, t) = \mathrm{e}^{-\mathbb{H}t}p(x, 0)$, with

$$\mathrm{e}^{-\mathbb{H}t} = \sum_\lambda \mathrm{e}^{-\lambda t}|r_\lambda\rangle\langle\ell_\lambda| \tag{4.35}$$

where r_λ refers to the eigenvectors of $\mathbb{H}$ with eigenvalue λ. Since $\mathbb{H}$ is not Hermitian, the λ's don't have to be real, and in general they won't be. The function ℓ_λ is the eigenvector of

$\mathbb{H}^\dagger$. Clearly, the eigenvalues λ have a strong physical meaning: their real parts form the set of relaxation rates that characterize the system's dynamics. When there exists a steady-state, it must correspond to $\lambda = 0$ (which is non-degenerate if the steady-state is unique). All other eigenvalues λ must have a positive real part. The lowest "excited" state of $\mathbb{H}$, that is the eigenstates whose corresponding λ has its real part the closet to 0. The reciprocal of its real part is the slowest time scale governing the relaxation to the steady-state. If $\Im(\lambda) \neq 0$ this tells us that there will be oscillations on top of exponential relaxation. In practice, starting from an initial state $p(x, 0)$ we have that

$$|p(t)\rangle = \mathrm{e}^{-\mathbb{H}t}|p(0)\rangle,\ \ p(x,t) = \sum_\lambda \mathrm{e}^{-\lambda t} r_\lambda(x) \int \mathrm{d}y \ell_\lambda(y) p(y,0) \tag{4.36}$$

and the λ's clearly form a family of relaxation rates.

4.1.5 A simple example

Consider a one-dimensional Brownian particle on a segment of length ℓ whose ends at $x = 0$ and $x = \ell$ are absorbing, which means that the particle dies when hitting these boundaries. We want to solve $\partial_t p = D\partial_x^2 p$ with the boundary condition $p(x = 0 \text{ or } \ell, t) = 0$. The quantity $S(t) = \int_0^\ell \mathrm{d}x p(x, t)$ is the probability that the particle has survived up until time t. Sometimes S is called a survival probability. In order to find S one first diagonalizes $\mathbb{H} = -D\partial_x^2$, which, in practice, means solving

$$D\partial_x^2\phi = -\lambda\phi,\ \phi(0,t) = \phi(\ell,t) = 0 \tag{4.37}$$

whose (orthonormalized, $\int_0^\ell \mathrm{d}x\phi_n(x)\phi_m(x) = \delta_{mn}$) solutions are $\phi_n(x) = \sqrt{2/\ell}\sin k_n x$, with $k_n = n\pi/\ell$, $n \in \mathbb{N}^*$, and the corresponding eigenvalue is $\lambda_n = Dk_n^2$. These functions can be used to express the initial condition $p(x, 0)$:

$$p(x,0) = \sum_{j\geq 1} c_j(0)\phi_j(x),\ c_n(0) = \int \mathrm{d}x\phi_n(x)p(x,0) \tag{4.38}$$

so that, for instance when $p(x, 0) = \delta(x - x_0)$ ($x_0 \in [0, \ell]$), we have $c_n(0) = \phi_n(x_0)$ and thus

$$p(x,t) = \sum_{n\geq 1} \phi_n(0)\phi_n(x)\mathrm{e}^{-\lambda_n t} \tag{4.39}$$

and at large times the largest negative eigenvalue dominates the summation:

$$p(x,t) \simeq \frac{2}{\ell}\sin k_1 x_0 \sin k_1 x \mathrm{e}^{-D\pi^2 t/\ell^2} \tag{4.40}$$

and thus

$$S(t) \simeq \frac{4}{\pi}\sin(\pi x_0/\ell)\mathrm{e}^{-D\pi^2 t/\ell^2} \tag{4.41}$$

For a Brownian particle on a segment $[0, \ell]$ with periodic boundary conditions, and a biased motion at velocity v, $\dot{r} = v + \sqrt{2D}\eta$, the spectrum of $\mathbb{H}$ is made of the $\lambda_k = Dk^2 + ivk$, where $k = 2\pi n/\ell$, $n \in \mathbb{Z}$. The steady-state is $p_{\mathrm{ss}}(x) = 1/\ell$ and the eigenvalue whose real part is the closest to zero is $D(2\pi/\ell)^2 + iv2\pi/\ell$ (the eigenfunctions are $\phi_k(x) = \frac{1}{\sqrt{\ell}}\mathrm{e}^{ikx}$).

For the case of a particle with reflecting boundary conditions diffusing without any bias, the local particle flux $j = -D\partial_x p$ must vanish at the two boundaries, which forces the eigenfunctions to be $\cos kx$, with $k = k_n = \frac{\pi n}{\ell}$, $n \in \mathbb{N}$, hence the relaxation to the uniform steady-state is governed by $\lambda_1 = D\frac{\pi^2}{\ell^2}$, which is smaller than $D\frac{4\pi^2}{\ell^2}$, hence it takes a bit longer with reflecting boundary conditions than it does with periodic boundary conditions to reach the uniform state $p(x) = \frac{1}{\ell}$.

4.1.6 Adjoint equation and first-passage time

Interestingly, one can actually show that the mean time $\tau(y, x)$ at which the first passage to location y occurs, when starting from x, for a process evolving through $\dot{r} \overset{0}{=} f + g\eta$, is a solution of

$$a^{(1)}(x)\partial_x\tau + \frac{1}{2}a^{(2)}(x)\partial_x^2\tau = -1 \tag{4.42}$$

with the boundary condition $\tau(x, x) = 0$.

For the mean first-passage time $\tau(x_2, x_1)$ to x_2 starting from x_1, we expect

$$\int_y \tau(x_2, y)p(y, 0|x_1, -\mathrm{d}t) + \mathrm{d}t = \tau(x_2, x_1) \tag{4.43}$$

which we can phrase as follows: the time that it takes to hit x_2 starting from x_1 is the time that it takes to hit y starting from x_1 in a time $\mathrm{d}t$, to which one must add $\mathrm{d}t$, and that is regardless of y. We have denoted by $p(x', t'|x, t)$ the probability to be at x' at time t' given that one started from x at time t. We can then use that

$$p(y, 0|x_1, -\mathrm{d}t) = p(y, \mathrm{d}t|x_1, 0) = \delta(x_1 - y) + \mathrm{d}t\partial_y(-f(y)\delta(x_1 - y)) + \frac{1}{2}\partial_y^2(g^2(y)\delta(y - x_1)) \tag{4.44}$$

which results in

$$(\mathbb{H}^\dagger)_{x,x_1}\tau(x_2, x) = 1,\ f(x_1)\partial_{x_1}\tau(x_2, x_1) + \frac{g^2(x_1)}{2}\partial_{x_1}^2\tau(x_2, x_1) = -1 \tag{4.45}$$

Interestingly, $\mathbb{H}^\dagger$ appears in this equation, as it does in most reasonings involving some sort of time-reversal. In this particular situation, we know ahead of time the time it takes to reach a target.

There are many applications of first passage times and probabilities to nonequilibrium and biophysical systems. One of them is described in [10] and it deals with the best strategy to efficiently find food.

4.2 Equilibrium and time-reversibility

4.2.1 Probability current

When we consider a Langevin equation of the form $\dot{x}_\mu \overset{0}{=} f_\mu + g_{\mu j}\eta_j$ the related probability current is $J_\mu(x,t) = \underbrace{f_\mu}_{a_\mu^{(1)}} p + \frac{1}{2}\partial_\nu(\underbrace{g_{\mu i}g_{\nu i}}_{a_{\mu\nu}^{(2)}} p)$. This is not exactly $\langle \dot{x}_\mu \rangle$, so it is not always easy to picture what J_μ is. What we know for sure is that in a steady-state, we must have $\partial_\mu J_\mu = 0$: the current is divergence free.

We have already noted that when $f_\mu = -\partial_\mu V$ and $g_{\mu i} = \sqrt{2T}\delta_{\mu i}$, namely for an equilibrium dynamics, the probability current $J_\mu = -\partial_\mu V p - T\partial_\mu p$ vanishes when p reaches its equilibrium value $p_{\text{eq}}(x) = \mathrm{e}^{-V(x)/T}/Z$. This suggests that an alternative way of defining equilibrium is by requiring that the probability current vanish. In the second example of subsection 4.1.5 where $p_{\text{ss}}(x) = \frac{1}{\ell}$ we have that $J = vp - D\partial_x p = vp = \frac{v}{\ell}$ and this current indeed vanishes only when there is not directed motion (when $v = 0$).

Let's look deeper into another example, that of an underdamped Langevin equation for a particle with a unit mass $m = 1$:

$$\dot{x} = v,\ \dot{v} = -\gamma v - \partial_x V + \sqrt{2\gamma T}\eta \tag{4.46}$$

with the related Fokker-Planck equation for $p(x, v, t)$:

$$\partial_t p = -v\partial_x p + \partial_v((\gamma v + \partial_x V)p) + \gamma T \partial_v^2 p \tag{4.47}$$

This is a local conservation equation in the two-dimensional (x, v) space,

$$\partial_t p = -\partial_x J_x - \partial_v J_v,\ \begin{cases} J_x = vp \\ J_v = -(\gamma v + \partial_x V)p - \gamma T\partial_v p \end{cases} \tag{4.48}$$

where $J_x = \langle \dot{x} \rangle$ is the real spatial current. In a stationary state, whether equilibrium or not, we have $\partial_x J_x + \partial_v J_v = 0$. However, we know that the dynamics of Eq. (4.46) describes some equilibrium dynamics, since its related entropy production, at fixed initial and final states, is given by

$$\Sigma = \ln \frac{\mathscr{P}[x]}{\mathscr{P}[x^{\mathrm{R}}]} = -\frac{1}{\gamma T}\int_0^{t_{\text{obs}}} (\ddot{x} + \partial_x V)\gamma \dot{x} = \left[\frac{\dot{x}^2}{2} + V(x)\right]_0^{t_{\text{obs}}} \tag{4.49}$$

which tells us that choosing as the initial state a Boltzmann distribution, the system remains at zero entropy production and is thus in equilibrium. Now, let's evaluate the current components,

$$J_x = vp = v\frac{\mathrm{e}^{-\beta H(x,v)}}{Z},\ H(x,v) = \frac{1}{2}v^2 + V(x) \tag{4.50}$$

is obviously nonzero, and neither is J_v:

$$J_v = -(\gamma v + \partial_x V)p - \gamma T\partial_v p = -\partial_x V \frac{\mathrm{e}^{-\beta H(x,v)}}{Z} \tag{4.51}$$

This is no big deal for several reasons: first, unless we insisted on defining equilibrium through the vanishing of probability currents, there is no contradiction with equilibrium. Second, mathematically speaking, the only thing we know is that the current is divergence free, so that it is in general defined up to a curl. If we add $\boldsymbol{\nabla}\times\mathbf{A}$ to $\mathbf{J}$ then of course the property $\boldsymbol{\nabla}\cdot\mathbf{J}=0$ is preserved. In the example above, the choice $\mathbf{A}=Tp\mathbf{e}_z$ works fine (where z is a third direction perpendicular to x and v):

$$J'_x = J_x + \partial_v(Tp),\ J'_v = J_v - \partial_x(Tp) \tag{4.52}$$

and of course $J'_x=0$, $J'_v=0$. What matters eventually is only the divergence of the current, or its net flux across some surface of phase space, not the individual components of the current.

4.2.2 Detailed balance

Our definition of equilibrium is based on the fact that there is no way to distinguish a time-forward trajectory from its time-reversed counterpart. On practice this means that the joint probability $p(x,t;x',t')$ of observing the position x' at t' and x at time $t>t'$, verifies

$$p(x,t;x',t') = p(x',t;x,t') \tag{4.53}$$

In a steady-state, we have that $p(x,t;x',t')=p(x,t|x',t')p_{\text{ss}}(x')$, so that we must also have the so-called detailed balance condition:

$$p(x,t|x',t')p_{\text{ss}}(x') = p(x',t|x,t')p_{\text{ss}}(x) \tag{4.54}$$

When this is the case one writes that $p_{\text{ss}}=p_{\text{eq}}$. That's a very special brand of steady-state distribution. It is interesting to see what detailed balance tells us for the evolution operator $\mathbb{H}$. For this, we consider t' and $t=t'+\Delta t$, with Δt very small:

$$(\underbrace{p(x,t'|x',t')}_{\delta(x-x')}+\Delta t\ \partial_t p(x,t|x',t')\big|_{t=t'}+\ldots)p_{\text{eq}}(x') = (p(x',t'|x,t')+\Delta t\ \partial_t p(x',t|x,t')\big|_{t=t'}+\ldots)p_{\text{eq}}(x) \tag{4.55}$$

Using that $\partial_t p(x,t|x',t')\big|_{t=t'}=-\mathbb{H}_x\delta(x-x')$ and we $\partial_t p(x',t|x,t')\big|_{t=t'}=-\mathbb{H}_{x'}\delta(x-x')$ we obtain

$$\mathbb{H}_x\delta(x-x')p_{\text{eq}}(x') = \mathbb{H}_{x'}\delta(x-x')p_{\text{eq}}(x) \tag{4.56}$$

This is a not a very transparent equality, but when translated into what it really means, namely

$$\int \mathrm{d}x\mathrm{d}x'\phi(x)\mathbb{H}_x\delta(x-x')p_{\text{eq}}(x')\chi(x') = \int \mathrm{d}x\mathrm{d}x'\phi(x)\mathbb{H}_{x'}\delta(x-x')p_{\text{eq}}(x)\chi(x') \tag{4.57}$$

where ϕ and χ are dummy functions, and using the definition of the Hermitian conjugate,

$$\int \mathrm{d}x\mathrm{d}x'\phi(x)\mathbb{H}_x\delta(x-x')p_{\text{eq}}(x')\chi(x') = \int \mathrm{d}x\mathrm{d}x'(\mathbb{H}_x^\dagger\phi(x))\delta(x-x')p_{\text{eq}}(x')\chi(x') \tag{4.58}$$

then we arrive at

$$p_{\text{eq}}(x')\mathbb{H}_x^\dagger\delta(x-x') = p_{\text{eq}}(x)\mathbb{H}_{x'}\delta(x-x')p_{\text{eq}}(x) \tag{4.59}$$

Put more simply, $\mathbb{H}^\dagger = p_{\rm eq}^{-1}\mathbb{H}p_{\rm eq}$.

This takes a simple form for an overdamped Langevin particle

$$\mathbb{H}\bullet = -T\partial_x^2\bullet - \partial_x(V'\bullet) = -T\mathrm{e}^{-\beta V}\partial_x\left(\mathrm{e}^{\beta V(x)}\partial_x\bullet\right) \tag{4.60}$$

which is such that

$$\mathbb{H}^\dagger\bullet = -T\mathrm{e}^{+\beta V}\partial_x\left(\mathrm{e}^{-\beta V(x)}\partial_x\bullet\right) \tag{4.61}$$

This also means that $\mathbb{H}_s = p_{\rm eq}^{-1/2}\mathbb{H}p_{\rm eq}^{1/2}$ is Hermitian, which can be checked explicitly:

$$\mathbb{H}_s = -T\partial_x^2 + U(x),\ U(x) = \frac{V'^2}{4T} - \frac{1}{2}V'' \tag{4.62}$$

In retrospect, we see that in equilibrium the spectrum is thus real and $\mathbb{H}_s$ can be diagonalized in an orthogonal basis.

For a particle evolving according to an overdamped Langevin dynamics in some *a priori* arbitrary force field $\mathbf{F}$, we have that

$$\dot{\mathbf{r}} = \mathbf{F} + \sqrt{2T}\boldsymbol{\eta},\ \ \partial_t p(\mathbf{r},t) = \partial_{\mathbf{r}}\cdot(\mathbf{F}p) + T\partial_{\mathbf{r}}^2 p = -\mathbb{H}p \tag{4.63}$$

If we denote by $p_{\rm ss}$ the stationary distribution and if we define $H[\mathbf{r}] = -\ln p_{\rm ss}(\mathbf{r})$, then the new operator $\mathbb{H}' = p_{\rm ss}^{-1/2}\mathbb{H}p_{\rm ss}^{1/2}$ reads

$$\mathbb{H}' = \underbrace{-T\partial_{\mathbf{r}}^2 + \partial_{\mathbf{r}}\cdot\mathbf{F} - \frac{1}{2}\mathbf{F}\cdot\partial_{\mathbf{r}}H - \frac{T}{4}(\partial_{\mathbf{r}}H)^2 + \frac{T}{2}\partial_{\mathbf{r}}^2 H}_{\text{Hermitian}} + (T\partial_{\mathbf{r}}H + \mathbf{F})\cdot\partial_{\mathbf{r}} \tag{4.64}$$

and it is obviously not Hermitian, unless $\mathbf{F} = -\partial_{\mathbf{r}}V$ is conservative, and then $H(\mathbf{r}) = \beta V(\mathbf{r})$ as expected in equilibrium.

4.2.3 Stochastic thermodynamics 101

Jarzynski, Crooks, and the first principle

Let's imagine the situation in which our system is subjected to an external potential $V(\mathbf{r},k)$ that depends on an extra parameter k that can experimentally be controled. We assume that our system in equilibrium at the initial time, when the parameter takes the value k_0. Then at $t=0$ we implement a prescribed time protocol for $k(t)$, when ends at time t_f with a value k_f.

For this protocol, we have $\langle\mathrm{e}^{-\Sigma}\rangle = 1$ and $\Sigma = -\beta(F(k_f)-F(f_0)) + \beta(V(t_f)-V(0)) - \beta\int \mathrm{d}t\dot{\mathbf{r}}\cdot\boldsymbol{\nabla}V$. If $V(\mathbf{r},k(t))$ depends on a parameter that is time-dependent, then we cannot write that $\dot{\mathbf{r}}\cdot\boldsymbol{\nabla} = \frac{\mathrm{d}V}{\mathrm{d}t}$, because

$$\dot{\mathbf{r}}\cdot\boldsymbol{\nabla}V = \frac{\mathrm{d}V}{\mathrm{d}t} - \dot{k}\partial_k V \tag{4.65}$$

which leads to $\Sigma = -\beta\Delta F + \beta \int \mathrm{d}t\dot{k}\partial_k V$ (with $\Delta F = F(k_f) - F(f_0)$). According to the first principle, $\mathrm{d}V = \delta W + \delta Q$ but here we have

$$\mathrm{d}V = \dot{\mathbf{r}} \cdot \boldsymbol{\nabla} V + \mathrm{d}k\partial_k V \tag{4.66}$$

with $\boldsymbol{\nabla} V = -\dot{\mathbf{r}} + \sqrt{2T}\boldsymbol{\eta}$ which is the force exerted by the thermostat on the particle. If we agree to call the work performed by that force the heat received by the system from the thermostat, namely,

$$\delta Q = \dot{\mathbf{r}} \cdot \boldsymbol{\nabla} V = \dot{\mathbf{r}} \cdot (-\dot{\mathbf{r}} + \sqrt{2T}\boldsymbol{\eta}) \tag{4.67}$$

and $\delta W = \mathrm{d}k\partial_k V$ is the work performed by the operator on the system, then the first principle is respected. Interestingly, $\Sigma = -\beta\Delta F + \beta W$ and $\langle \mathrm{e}^{-\Sigma}\rangle = 1$ means that

$$\langle \mathrm{e}^{-\beta W}\rangle = \mathrm{e}^{-\beta\Delta F} \tag{4.68}$$

This is Jarzynski's equality [60]. One can similarly prove Crooks identity [25, 26] for the probabilitt $P(W)$ that a work W is performed. This is done by marginalizing the probability of a trajectory and using that upon time reversal W becomes $-W$:

$$P(W) = P(-W)\mathrm{e}^{\beta W - \beta\Delta F} \tag{4.69}$$

Of course, the Kullback-Leibler divergence being positive means that $\langle \Sigma \geq 0$, but since $\Sigma = -\beta\Delta F + \beta \int \mathrm{d}t\dot{k}\partial_k V = -\beta\Delta F + \beta W$ this means that

$$\langle W\rangle \geq \Delta F \tag{4.70}$$

which is a well-known formulation of the second-principle of thermodynamics [61] (in macroscopic thermodynamics, for an isothermal reversible transformation $\Delta F = W_{\text{rev}}$). This seems to endow $\langle\Sigma\rangle$ with the meaning of a total entropy variation. Let's have a closer look.

Entropy balance

Our goal is now to explore the extent to which we can build a fluctuating observable called entropy the average of which would be a standard entropy verifying the second principle for a particle with overdamped Langevin dynamics $\dot{\mathbf{r}} = \mathbf{F} + \sqrt{2T}\boldsymbol{\eta}$. To do this, we introduce $\hat{S}(t) = -\ln p(\mathbf{r}(t), t)$ which is, for now, a strange fluctuating quantity. However, it is clear that $\langle \hat{S}\rangle = S$ is the Shannon entropy corresponding to $p(\mathbf{x}, t)$ (which is identical to the entropy in equilibrium). Using Stratonovich calculus, we see that

$$\begin{aligned}
\frac{\mathrm{d}\hat{S}}{\mathrm{d}t} &\overset{1/2}{=} -\frac{\partial_t p}{p} - \frac{\boldsymbol{\nabla} p}{p}\dot{\mathbf{r}} \\
&\overset{1/2}{=} -\frac{\partial_t p}{p} - \frac{\boldsymbol{\nabla} p}{p}\left(\mathbf{F} + \sqrt{2T}\boldsymbol{\eta}\right) \\
&\overset{1/2}{=} -\frac{\partial_t p}{p} - \frac{\boldsymbol{\nabla} p}{p}\cdot\mathbf{F} - \sqrt{2T}\frac{\boldsymbol{\nabla} p}{p}\cdot\boldsymbol{\eta} \\
&\overset{0}{=} -\frac{\partial_t p}{p} - \frac{\boldsymbol{\nabla} p}{p}\cdot\mathbf{F} - T\nabla\left(\frac{\boldsymbol{\nabla} p}{p}\right) - \sqrt{2T}\frac{\boldsymbol{\nabla} p}{p}\cdot\boldsymbol{\eta}
\end{aligned} \tag{4.71}$$

hence, upon averaging, we get

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \int \mathrm{d}^d r \left[-\frac{\boldsymbol{\nabla} p}{\cdot}\mathbf{F} - Tp\nabla\left(\frac{\boldsymbol{\nabla} p}{p}\right)\right] \tag{4.72}$$

and using that $\mathbf{j} = \mathbf{F}p - T\boldsymbol{\nabla} p$ we can replace $\boldsymbol{\nabla} p$ with $\frac{\mathbf{F}p-\mathbf{j}}{T}$ and proceed with an integration par parts:

$$\begin{aligned}\frac{\mathrm{d}S}{\mathrm{d}t} &= \int \mathrm{d}^d r \left[-\frac{\mathbf{F}p - \mathbf{j}}{T}\cdot \mathbf{F} + \frac{(\mathbf{F}p-\mathbf{j}^2}{pT}\right] \\ &= \int \mathrm{d}^d r \left[\frac{\mathbf{j}^2}{Tp} - \frac{1}{T}\mathbf{F}\cdot\mathbf{j}\right]\end{aligned} \tag{4.73}$$

Of course this is compatible with the previous approach according to which $\Sigma = \hat{S}(t_{\text{obs}}) - \hat{S}(0) - \frac{1}{T}\int \mathrm{d}t\mathbf{F}\cdot\dot{\mathbf{r}}$. We have already argued that $-\mathbf{F}$ is also the force exerted by the thermostat on the system, and thus that $\int \mathrm{d}t\mathbf{F}\cdot\dot{\mathbf{r}}$ can be seen as work done by the system on the thermostat, which is also the heat exchanged and thus that $\Delta\hat{S}_{\text{ext}} = \frac{1}{T}\int\mathrm{d}t\mathbf{F}\cdot\dot{\mathbf{r}}$ can be seen as the entropy exchanged with the external medium. In that sense, $\Sigma = \Delta\hat{S}_{\text{global}}$ is the variation of the total entropy, and thus

$$\Delta\hat{S}_{\text{global}} = \Sigma = \Delta\hat{S} + \Delta\hat{S}_{\text{ext}} \tag{4.74}$$

We already know that $\langle\Sigma\rangle \geq 0$ so that, upon averaging

$$\Delta S + \Delta S_{\text{ext}} \geq 0 \tag{4.75}$$

with an equality only if the transformations are reversible. In a nonequilibrium stationary state, $\Delta S = 0$ and thus $\langle\Sigma\rangle = \Delta S_{\text{global}} = \Delta S_{\text{ext}} > 0$ is the entropy production.

Within the framework of Langevin dynamics, $\langle\Sigma\rangle$ can be seen to take a simple form:

$$\frac{\mathrm{d}S_{\text{global}}}{\mathrm{d}t} = \int \mathrm{d}x\frac{\mathbf{j}^2}{Tp} = \frac{\mathrm{d}S_i}{\mathrm{d}t} \tag{4.76}$$

4.2.4 Linear response and the fluctuation-dissipation theorem

Consider an overdamped equilibrium dynamics for a particle with position x in some external potential $V(x)$ (we work in $d = 1$ to make notations lighter), that has reached equilibrium for a long time, whose evolution is

$$\dot{x} = -V' + f + \sqrt{2T}\eta \tag{4.77}$$

where f is an infinitesimal small perturbing force that acts as of time $t' > 0$. And we ask about how a quantity $B(x(t)) = B(t)$ responds,

$$R(t,t') = \left.\frac{\delta\langle B(t)\rangle}{\delta f(t')}\right|_{f=0} \tag{4.78}$$

with

$$\langle B\rangle = \int \mathscr{D}xB(x(t))\mathrm{e}^{-\frac{1}{4T}\int\mathrm{d}s(\dot{x}+V'-f)} \tag{4.79}$$

so that

$$R(t,t') = \frac{1}{2T}\langle B(x(t))(\dot{x} + V')(t')\rangle \tag{4.80}$$

and in a similar fashion

$$R(-t,-t') = \frac{1}{2T}\langle B(x(-t))(\dot{x} + V')(-t')\rangle \tag{4.81}$$

so that

$$R(t,t')-R(-t,-t') = \frac{1}{2T}\left[\langle B(x(t))\dot{x}(t') - B(x(-t))\dot{x}(-t')\rangle\right]+\frac{1}{2T}\langle B(x(t))\,V'(x(t'))-B(x(-t))\,V'(x(-t'))\rangle \tag{4.82}$$

At this stage we use that in equilibrium the dynamics is time-reversible so that $\langle B(x(t))\,V'(x(t'))-B(x(-t))\,V'(x(-t'))\rangle = 0$ while

$$\langle B(x(t))\dot{x}(t') - B(x(-t))\dot{x}(-t')\rangle = 2\frac{\mathrm{d}}{\mathrm{d}t'}\langle B(x(t))\dot{x}(t')\rangle \tag{4.83}$$

which again leads to $R(\tau) - R(-\tau) = -\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}\tau}\langle B(\tau)x(0)\rangle$.

The entropy production rate in the presence of an external force f that drives the system out of equilibrium is given by

$$\sigma = \frac{1}{T}\langle \dot{x}f\rangle = \lim_{t\to 0}\frac{\mathrm{d}}{\mathrm{d}t}\left[TR(t) + \dot{C}(t)\right] \tag{4.84}$$

which is the Harada-Sasa equality (the proof that can be found here [53, 54] is a bit tricky). Here R and C are the position response and the position auto-correlation function.

4.3 A tiny bit of optimal transport

Consider an overdamped Brownian particle with position $\mathbf{r}(t)$ in an external potential $V(\mathbf{x},t)$ that depends on time and that is controled by the operator. At the initial time, the potential is $V_0(\mathbf{x}) = V(\mathbf{x},0)$ and the particle is assumed to be in thermal equilibrium with a Boltzmann distribution $\rho_0(\mathbf{x}) = \frac{\mathrm{e}^{-\beta V_0(\mathbf{x})}}{Z_0}$. Our goal is to tune and adjust the external potential $V(\mathbf{x},t)$ so that at the final observation time t_{obs}, the particle is distributed according to $\rho_1(\mathbf{x}) = \frac{\mathrm{e}^{-\beta V_1(\mathbf{x})}}{Z_1}$, where ρ_1 (or, equivalently, V_1), is prescribed. However, we want to achieve this procedure by dissipating the least possible energy into the environment. The Langevin equation for the particle reads

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu\boldsymbol{\nabla} V(\mathbf{r}(t),t) + \sqrt{2\mu T}\boldsymbol{\eta} \tag{4.85}$$

where μ is the particle's mobility and the components of $\boldsymbol{\eta}$ are independent Gaussian white noises with correlations $\langle \eta^\alpha(t)\eta^{\alpha'}(t')\rangle = \delta^{\alpha\alpha'}\delta(t-t')$ ($\alpha,\alpha' = 1,\dots,d$, d being the space dimension). The probability density to find the particle at position $\mathbf{r}(t) = \mathbf{x}$ at time t is denoted by $\rho(\mathbf{x},t)$.