16. Working with the Langevin and Fokker-Planck equations

In the preceding Lecture, we have shown that given a Langevin equation (LE), it is possible to write down an equivalent Fokker-Planck equation (FPE), which is a partial differential equation to study the time evolution of the probability distribution function, i.e. of the function which measures the probability that our particle moving in a 1D potential is in the position x at time t.

In this Lecture, we study some particular examples of 1D dynamics, and we show how to handle the Langevin and Fokker-Planck equations to study the steady states and the dynamics of a stochastic system.

16.1. Steady state solutions and the fluctuation-dissipation theorem

Let us consider the Langevin equation to describe the approach to thermodynamic equilibrium of a particle in a potential V,

$$\frac{dx}{dt} = -\frac{1}{\gamma}\frac{\partial V}{\partial x} + \sqrt{2D}\eta(t). \tag{1}$$

The equivalent FPE is then:

$$\frac{\partial P(x,t)}{\partial t} = \frac{1}{\gamma}\frac{\partial}{\partial x}\left[\frac{\partial V(x)}{\partial x}P(x,t)\right] + D\frac{\partial^2 P(x,t)}{\partial x^2} \tag{2}$$

where we have called $P(x,t) \equiv P(x,t;x_0,t_0)$, i.e. dropping out the dependence on the initial condition for simplicity. The steady state solution is such that $\frac{\partial P(x,t)}{\partial t} = 0$.

If we call the steady state probability distribution $P_s(x)$, the equation for $P_s(x)$ may be rewritten as:

$$\frac{\partial}{\partial x}\left[\frac{1}{\gamma}\frac{\partial V(x)}{\partial x}P_s(x) + D\frac{\partial}{\partial x}P_s(x)\right] \equiv \frac{\partial}{\partial x}J(x) = 0, \tag{3}$$

where J denotes the probability "flux". J therefore needs to be a constant. On the other hand, we need the probability and the moments of P to be finite, and this requires P to decay "fast" at infinity (specifically, faster than $|x|^{-n-1}$ if the moments up to the $n-$th are finite). In particular both $P_s(x)$ and $\frac{\partial}{\partial x}P_s(x)$ are 0 at infinity, and therefore J is 0 at infinity. As it needs to be constant, the only possible solution is that it is 0 everywhere. Therefore, the equation for $P_s(x)$ becomes:

$$\frac{1}{\gamma}\frac{\partial V(x)}{\partial x}P_s(x) + D\frac{\partial}{\partial x}P_s(x) = 0, \tag{4}$$

which is readily solved by:

$$P_s(x) \propto \exp\left(-\frac{V(x)}{\gamma D}\right) \tag{5}$$

is the steady state solution. In order for this result to be compatible with the known equilibrium distribution, $P(x) = \exp(-\beta V(x))$, we re-obtain the

Einstein relation $D = k_B T \Gamma$. In general this procedure leads to the existence of a fluctuation-dissipation theorem analogous to the one proved in Lecture 14 for a sphere in water.

As an exercise, you can consider the Langevin equation:

$$m\frac{dv}{dt} = -\gamma v + \frac{\sqrt{2k_B T\gamma}}{m}\eta(t) \tag{6}$$

with $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$. Show that the stationary distribution is the Maxwellian.

16.2. Time-dependent calculations: a particle in a potential well

Let us now see an example of time dependent calculations (i.e. we see how to handle the Langevin and Fokker-Planck equations when we are *not* in steady state).

Consider a particle moving in a 1D Harmonic potential, $V(x) = \alpha x^2/2$, so that its Langevin equation is:

$$\frac{dx}{dt} = -\frac{\alpha x}{\gamma} + \sqrt{2D}\eta(t), \tag{7}$$

with $\eta(t)$ as usual a Gaussian random noise. The associated Fokker-Planck equation is:

$$\frac{\partial}{\partial t}P = \frac{\alpha}{\gamma}\frac{\partial}{\partial x}xP + D\frac{\partial^2}{\partial x^2}P. \tag{8}$$

The particle starts at x_0.

Note that the Langevin equation has the same form as the one considered in 14.1, and therefore we could use that procedure. Here we want to use the Fokker-Plank equation. First, let us write down an equation for $\langle x(t)\rangle$. To do so, we multiply both sides of Eq. 8 by x, and integrate over all possible values of x:

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty} dx x P(x,t) = \frac{\alpha}{\gamma}\int_{-\infty}^{+\infty} dx x \frac{\partial}{\partial x} x P(x,t) + \sqrt{2D}\int_{-\infty}^{+\infty} dx x \frac{\partial^2}{\partial x^2} P(x,t). \tag{9}$$

We can now integrate by parts the terms in the right hand side. As $P(x,t)$ is normalisable and its moments (at least up to the second), are well defined, this means that P decays "fast enough" at infinity, hence the boundary terms in the integration by parts vanish. As a result we are left with the following equation for the first moment:

$$\frac{d\langle x(t)\rangle}{dt} = -\frac{\alpha}{\gamma}\langle x(t)\rangle, \tag{10}$$

which is easily solved by:

$$\langle x(t)\rangle = x_0 \exp\left(-\frac{\alpha t}{\gamma}\right). \tag{11}$$

We can write down an equation for the second moment in a similar way, by multiplying both sides of the Fokker-Planck equation by x^2 and then integrating by parts. This time the diffusive term also contributes as the second derivative $d^2/dx^2 x^2 = 2$ is also non-zero. Let us also now specialise to the case $x_0 = 0$. We end up with the following equation:

$$\frac{d\langle x^2(t)\rangle}{dt} = -2\frac{\alpha}{\gamma}\langle x^2(t)\rangle + 2D, \tag{12}$$

which is again standard, and solved by ($\langle x^2(0)\rangle = 0$ as $P(x, t = 0) = \delta(x - x_0) = \delta(x)$):

$$\langle x^2(t)\rangle = \frac{D\gamma}{\alpha}\left[1 - \exp\left(-\frac{2\alpha t}{\gamma}\right)\right]. \tag{13}$$

The limits of Eq. 13 for small and large times are noteworthy. As $t \to 0$, we obtain $\langle x^2(t)\rangle \sim 2Dt$, so that the particle performs an unrestricted random motion. This is because at early times the particle does not "feel" the presence of the potential and it just diffuses around (as it starts from the minimum of the potential). At large times, on the other hand, $\langle x^2(t)\rangle$ is finite and equal to $\frac{D\gamma}{\alpha}$, as the confining potential limits the fluctuations. The particle is undergoing small Brownian fluctuations close to the minimum of the potential well.

16.3. Steady state for multiplicative noise

Let us now turn to the more complicated case in which the term multiplying the stochastic term $\eta(t)$ in the Langevin equation is not a constant anymore. This case if often referred to as "multiplicative noise". In practice, this arises for instance when the system has absorbing states (i.e. sinks for the dynamics from where the system cannot escape – note that this is a clear violation of ergodicity). Consider then the Langevin equation:

$$\frac{dx}{dt} = f(x(t)) + g(x(t))\eta(t). \tag{14}$$

The associated Fokker-Planck is:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[(f(x)P(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[\frac{g(x)^2}{2}P(x,t)\right]. \tag{15}$$

Let us consider the specific case of a double well with stochastically varying barrier curvature, i.e.

$$f(x) = ax - bx^3 \tag{16}$$

$$g(x) = Qx \tag{17}$$

with $a, b, Q > 0$. The strength of Q is arbitrary as we imagine that the system is far from equilibrium. Indeed you can see that $x = 0$ is what is called an "absorbing state", as if the system is in 0 it never leaves it (because there is no noise there). This then blatantly violates the fluctuation-dissipation theorem so that the system needs to be far from equilibrium.

The steady state solution of Eq. 15 can be found by using a similar method as the one used in 16.1, by defining a flux which is constant and 0 at infinity. This time it is useful to call $Y(x) = g^2(x)P_s(x)$ and solve for Y in the resulting first order differential equation (try it and see why!). If we do that, we find that the steady state solution of the Fokker-Planck equation is:

$$P(x) \sim \frac{1}{g(x)^2} \exp\left(\int^x \frac{f(x')}{g(x')^2/2} dx' \right) \tag{18}$$

$$\sim \frac{1}{x^2} \exp\left[\int^x (2a/(Q^2 x') - 2bx'/Q^2) dx' \right] \tag{19}$$

$$\sim \exp\left[2\left(\frac{a}{Q^2} - 1 \right) \log x - bx^2/Q^2 \right]. \tag{20}$$

It is interesting to compute the maxima of the steady state distribution in Eq. 18. These are the values, x^*, which are most likely to be observed in a trial experiment and are defined through the equations:

$$\left(\frac{dP}{dx} \right)_{x=x^*}, \qquad \left(\frac{d^2P}{dx^2} \right)_{x=x^*} < 0. \tag{21}$$

From Eq. 18, we obtain that the derivative of the steady state probability distribution is 0 at:

$$(x^*)^2 = \frac{a - Q^2}{b} \tag{22}$$

In other words x^* depends on the strength of noise and reduces to the extrema of the double well potential only when the noise strength is sent to 0 (deterministic limit) !! This is an important result which shows that this kind of multiplicative "nonequilibrium" noise (ie violating the fluctuation-dissipation theorem) in general even affects the "equilibria" of a potential system. As a consequence, for instance a dynamical system with multiplicative noise exhibiting a bifurcation may be driven past the threshold by tuning the strength of the noise alone. This would never happen with a system obeying the fluctuation-dissipation theorem (and with constant g). In that case increasing the importance of the noise strength is equivalent to raising the temperature, so that all what happens is that there are more frequent hops between the minima of the potentials, but the probability in steady state would always be $\propto \exp(-\beta V(x))$, so that its maxima would always (for all values of T hence β) be those of the potential $V(x)$.

16.4. Time-dependent calculations: mean first passage times and Kramer problems*

We now discuss the computation of first and mean first passage times within the FPE formalism. This is an important example of a *dynamic* problem, i.e.

one in which the FPE at times smaller than ∞ (steady state) is the quantity we are interested in. *First passage times* problems are common and useful in a variety of context (e.g. to find the time needed for reactants to find each other in a reaction-diffusion equation, or the time necessary for a particle to escape a potential well – i.e. Kramers' problem, or the time needed for a stock market to recover its pre-crash status).

First passage problems may be introduced as follows. Take for instance a particle undergoing a 1D random walk (in the presence or absence of a thermodynamic potential). We are interested in calculating the time that it takes it to reach a point x (or a boundary A) *for the first time*, and we denote this quantity by $T(x)$ (for instance, if the particle is a man sleep-walking – which we might model via a random walk – on a roof, a natural choice for x is the edge of the roof...). $T(x)$ is the *first passage time* at x, and it is associated with a probability density $f(x,t)$, which gives the probability that x is reached at time t. In order to calculate $f(x,t)$ and its moments, we need to solve the associated FPE for $P(x,t;x_0,t_0)$, with absorbing boundary conditions in A:

$$P(x,t) = 0 \ \forall x \in A \, , \, \forall t \tag{23}$$

Let us write for convenience the FPE as:

$$\frac{\partial P}{\partial t} = \vec{\nabla} \cdot \left(\vec{J} \right) = LP. \tag{24}$$

We may also introduce any number of reflecting boundaries. At a reflecting boundary B, there is zero flux:

$$\vec{J} \cdot \hat{n} = 0 \tag{25}$$

where $\hat{n}$ is the unit vector normal to B. This corresponds for instance to a random walker being reflected after hitting the boundary at B. Let us further assume the initial condition that the particle is initially at x_0:

$$P(\vec{x},0) = \delta(\vec{x} - \vec{x}_0). \tag{26}$$

We denote by $T(\vec{x}_0)$ the first passage time from $\vec{x}_0$ to A. The probability that at time t the absorbing boundary A has not yet been reached is called the *survival probability*, $S(\vec{x}_0,t)$, while the probability that the absorbing boundary is reached at time t is denoted by $f(\vec{x}_0,t)$. We can thus write:

$$S(\vec{x}_0,t) = \int d\vec{x} P(\vec{x},t;\vec{x}_0,0), \tag{27}$$

$$S(\vec{x}_0,t) = \text{Prob } (T(\vec{x}_0) > t) = \int_t^\infty f(\vec{x}_0,t)dt, \tag{28}$$

$$f(\vec{x}_0,t) = -\frac{\partial S(\vec{x}_0,t)}{\partial t}. \tag{29}$$

If one is interested in the low moments of T, $\langle T^n \rangle$, rather than in the full distribution $f(\vec{x}_0,t)$, the analysis simplifies significantly, and we can write down a hierarchy of equations to determine them. In particular we can write (we will typically henceforth drop the dependence on $\vec{x}_0$ for readability):

$$\begin{aligned} \langle T^n \rangle &= \int_0^\infty t^n f(\vec{x}_0, t) && (30) \\ &= -\int_0^\infty t^n S'(t) dt && (31) \\ &= t^n \left(S(\infty) - S(0) \right) + n \int_0^\infty t^{n-1} S(t) dt, && (32) \end{aligned}$$

and $(S(\infty) - S(0)) = 0$ for $S(t)$ to be a well-behaved pdf. Note that in particular one has:

$$\langle T \rangle = \int_0^\infty S(t) dt. \tag{33}$$

Trading the integrals over time with integrals over space we obtain:

$$\begin{aligned} \langle T^n \rangle &= \int_0^\infty S(t) t^{n-1} dt = n \int d\vec{x} g_{n-1}(\vec{x}; \vec{x}_0) && (34) \\ g_n(\vec{x}; \vec{x}_0) &= \int_0^\infty t^n P(\vec{x}, t; \vec{x}_0, 0) dt, && (35) \end{aligned}$$

i.e. $g_n(\vec{x}; \vec{x}_0)$ gives the $n-$th moment in time of the probability of finding the particle at $\vec{x}$, given that it started in $\vec{x}_0$.

Now, starting from a time integral of t^n times the FPE and integrating by parts, we obtain:

$$\begin{aligned} \int t^n \frac{\partial P(\vec{x}, t; \vec{x}_0, 0)}{\partial t} dt &= t^n \left(P(t \to \infty) - P(t = 0) \right) && (36) \\ &- n \int dt t^{n-1} P(\vec{x}, t; \vec{x}_0, 0) \\ &= L \int_0^\infty dt t^n P(\vec{x}, t; \vec{x}_0, 0). && (37) \end{aligned}$$

The functions $g_n(\vec{x}; \vec{x}_0)$ thus satisfy the following hierarchy of PDEs:

$$\begin{aligned} L g_0(\vec{x}, \vec{x}_0) &= -\delta(\vec{x} - \vec{x}_0) && (38) \\ &\cdots \\ L g_n(\vec{x}, \vec{x}_0) &= -g_{n-1}(\vec{x}; \vec{x}_0), && (39) \end{aligned}$$

where we have used the facts that $P(t = 0) = \delta(\vec{x} - \vec{x}_0)$ due to the initial condition, and that

$$t^n \left(P(t \to \infty) - P(t = 0) \right) = 0 \tag{40}$$

for $n > 0$ due to the existence of the $n - th$ moment. The boundary conditions for the equations obeyed by the g_n's are $g_n = 0$ on the absorbing boundary A and $\vec{J}_n \cdot \hat{n} = 0$ on the reflecting boundaries ($\vec{\nabla} \cdot J_n = -\frac{\partial g_n}{\partial t}$).

Example 1. First passage time for a 1D biased random walker

As an example we consider the case of a 1D biased random walker, moving in $x > 0$ with a diffusion coefficient D and against a force f (which is directed along the negative x axis). Show that its FPE is:

$$\frac{\partial P}{\partial t} = \frac{f}{\gamma}\frac{\partial P}{\partial x} + D\frac{\partial^2 P}{\partial x^2}. \tag{41}$$

We now want to compute the first passage time at δ, starting from a point x, $0 < x < \delta$. So the quantity we are interested in is:

$$\tau(x) \equiv \langle T(x)\rangle = \int dx' g_0(x', x). \tag{42}$$

You may show that $\tau(x)$ obeys the following partial differential equation:

$$-\frac{f}{\gamma}\frac{\partial \tau(x)}{\partial x} + D\frac{\partial^2 \tau(x)}{\partial x^2} = -1 \tag{43}$$

with boundary conditions:

$$\left(\frac{\partial \tau(x)}{\partial x}\right)_{x=0} = 0 \tag{44}$$

$$\tau(x = \delta) = 0. \tag{45}$$

Eq. 43 can be solved by using the standard methods for (second-order inhomogeneous) ODEs. Verify that its solution is:

$$\tau(x) = \frac{\gamma^2 D}{f^2}\left[\exp\left(\frac{f\delta}{\gamma D}\right) - \exp\left(\frac{fx}{\gamma D}\right) + \frac{\gamma(x-\delta)}{f}\right] \tag{46}$$

$$\int_0^\delta \tau(x)dx = \frac{\delta^2}{D}\frac{e^\omega - 1 - \omega}{\omega^2}, \tag{47}$$

where $\omega \equiv \frac{f\delta}{\gamma D} = \frac{f\delta}{k_B T}$. It can be noted that for $f = 0$ (unbiased random walk), the first passage time to get to δ is $\delta^2/(2D)$, as expected from the theory of random walks.