

1/ We introduce the intensity and the phase : $E_x = A \cos \theta$ and $E_y = A \sin \theta$. Write the SDE for $A(t)$ and $\theta(t)$ within the Stratonovich convention. What can you do next ?

2/ We write $E_x + i E_y = A e^{i\theta} = e^{\lambda + i\theta}$.

Using Itô calculus, express $d\lambda + i d\theta$ as a function of λ , θ and the noises $dW_x(t)$ and $dW_y(t)$. Show that

$$dW_A(t) = \cos \theta(t) dW_x(t) + \sin \theta(t) dW_y(t) \text{ and } dW_\theta(t) = -\sin \theta(t) dW_x(t) + \cos \theta(t) dW_y(t) \quad (3.67)$$

are two independent noises. Deduce two Itô SDE for $\lambda(t)$ and $\theta(t)$ involving these new noises.

3/ Using the Itô formula, deduce the Itô SDE for the amplitude $A = |E_x + i E_y|$. Compare the related Stratonovich SDE for A to the one obtained in the question 1/. Discuss

4/ Write the SDE for the amplitude under the form

$$dA(t) = -V'(A(t)) dt + \sqrt{D} dW_A(t) \quad (3.68)$$

and give the “potential” $V(A)$. Find its minimum and plot $V(A)$.

5/ Write the FPE related to the SDE for $A(t)$. Deduce the stationary distribution. Discuss the distribution of the intensity $I = A^2$. Compute $\langle I \rangle$ and $\sqrt{\langle I^2 \rangle_c}$.

4 Stochastic processes (4) : the Fokker-Planck approach

When studying a stochastic process, the main goal is to determine its statistical properties, i.e. in particular its distribution. The Langevin approach (SDE) provides a natural way to approach the problem, as it starts from the microscopic stochastic time evolution usually at the root of a model. It is sometimes a suitable starting point for numerical simulations, however the statistical analysis comes in a second step. Within the Fokker-Planck approach, emphasis is already on the distribution since the Fokker-Planck equation (FPE) governs the time evolution of the distribution, hence is a prominent tool. In this chapter, we discuss several applications of the FPE and will demonstrate the power of the approach, compared to the SDE approach : we will see that it is more appropriate in order to address subtle properties like exit problem or first passage time analysis.

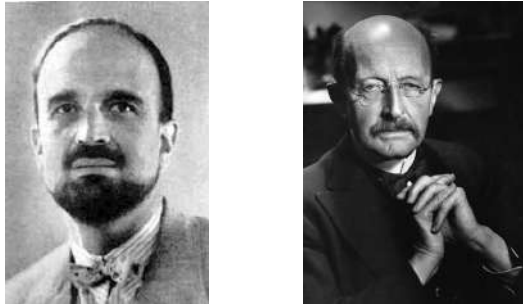


Figure 4.1: Adriaan Fokker (1887-1972) and Max Planck (1858-1947)

Jump process *versus* diffusion

In general, the master equation can be written under the form

$$\partial_t P_t(x) = \mathcal{L} P_t(x) \quad (4.1)$$

where $\mathcal{L}$ is a linear operator.

- For a *jump process*, the linear operator is an integral operator. For example, a simple **jump process** is the CPP studied above, for which $[\mathcal{L}\varphi](x) = \lambda \int d\eta w(\eta)(\varphi(x-\eta) - \varphi(x))$. In the general case, the distribution $w(\eta)$ of the jump amplitude and the jump rate depend on the initial position, hence a more general form of integral kernel (with no translation invariance) is $[\mathcal{L}\varphi](x) = -\lambda(x)\varphi(x) + \int d\eta \lambda(x-\eta) w(x-\eta; \eta) \varphi(x-\eta)$ (here $\lambda(x)$ the jump rate from x and $w(x; \eta)$ is the distribution of jump amplitude η from x).
- If the linear operator is a differential operator, $\mathcal{L} = -\partial_x F(x) + \partial_x^2 D(x)$, one says that the process is “**a diffusion**”. From the Pawula theorem, the differential operator can be at most second order. Physically, a diffusion is obtained as the limit of small jumps occurring with high rate. This is the type of stochastic processes discussed in the previous chapter on SDE and the present one on FPE.
- In general, a Markov process can combine a diffusion and jumps.

In this chapter, we only discuss diffusions.

4.1 Interpretation of the Fokker-Planck equation

The FPE describes a specific class of stochastic processes (called “*diffusions*”) for which the integro-differential master equation (2.26) can be reduced to a differential equation :

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial}{\partial x} [F(x) P_t(x)] + \frac{\partial^2}{\partial x^2} [D(x) P_t(x)] \quad (4.2)$$

(in the most general case, we could consider time dependent drift $F(x, t)$ and diffusion $D(x, t)$). Below, we explain precisely within what limits and under what conditions we can go from (2.26) to (4.2). The equation is also known as the “*Kolmogorov equation*” or, for $D(x) \rightarrow D$, the “*Smoluchowski equation*”. Let us first give the interpretation of the two terms in the Fokker-Planck equation (applications will be discussed below).

a) Drift : effect of the energy

Imagine that only the first term is present and that $F(x) \rightarrow F$ is uniform, we get

$$\frac{\partial P_t(x)}{\partial t} = -F \frac{\partial P_t(x)}{\partial x}. \quad (4.3)$$

The general solution is $P_t(x) = \varphi(x - Ft)$, where $P_0(x) = \varphi(x)$ is the initial distribution, thus F is the velocity (for uniform F , there is no deformation of the distribution) : Fig. 4.2. The first term in (4.2) is the **drift term**, where “the drift” $F(x)$ is interpreted as the force acting on the particle (remember that velocity=force). This is an effect of the energy as the force derives from a potential energy (at least in 1D).

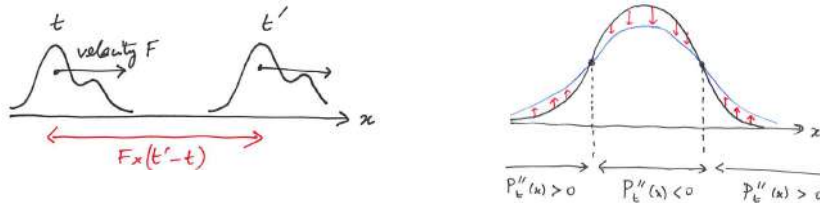


Figure 4.2: Left : *effect of drift*. Right : *the spreading of the distribution due to the diffusion term*.

b) Diffusion : effect of the entropy

Consider now the effect of the second term of (4.2) for a uniform $D(x) \rightarrow D$.

$$\frac{\partial P_t(x)}{\partial t} = D \frac{\partial^2 P_t(x)}{\partial x^2}. \quad (4.4)$$

As t grows, the distribution increases where the function is convex and diminishes where the function is concave (Fig. 4.2). This leads to a spreading of the distribution. The second term in (4.2) is the **diffusion term**, $D(x)$ playing the role of a x -dependent diffusion constant. This is an entropic effect (density tends to homogeneize).

c) Current density

The Fokker-Planck equation can be rewritten under the form of a **conservation equation**

$$\frac{\partial P_t(x)}{\partial t} = - \frac{\partial J_t(x)}{\partial x} \quad (4.5)$$

where

$$J_t(x) = \underbrace{F(x) P_t(x)}_{\text{drift current}} - \underbrace{\frac{\partial}{\partial x} [D(x) P_t(x)]}_{\text{diffusion current}} \quad (4.6)$$

is the current density. The drift current is the usual velocity $\times$ density. The diffusion term accounts for the fact that when the density is not uniform, particles move from high density regions to low density regions in order to homogenize the density (entropic effect).

d -dimensional case : the FPE reads $\partial_t P_t(\vec{x}) = -\partial_i [F_i(\vec{x}) P_t(\vec{x})] + \partial_i \partial_j [D_{ij}(\vec{x}) P_t(\vec{x})]$ where $\partial_i \equiv \partial/\partial x_i$ and D_{ij} is the (anisotropic) symmetric diffusion tensor. The conservation equation takes the form $\partial_t P_t(\vec{x}) = -\text{div} \vec{J}(\vec{x}, t)$, where the current density is now a vectorial field

$$J_i(\vec{x}, t) = F_i(\vec{x}) P_t(\vec{x}) - \partial_j [D_{ij}(\vec{x}) P_t(\vec{x})]. \quad (4.7)$$

Current has dimension $[J] = L^{1-d}/T$ (in 1D this is a current, however in $d > 1$ it is a current density).

Remark : The (uniform) diffusion constant D is the coefficient between the density gradient and the diffusion current, $J_t^{(\text{diff})}(x) = -D \partial_x P_t(x)$. When the diffusion constant depends on x , a natural generalization of the diffusion current, which can be preferred to (4.6), is

$$J_t(x) = \tilde{F}(x) P_t(x) - D(x) \partial_x P_t(x) \quad (4.8)$$

the two terms being interpreted as contributions from drift and diffusion, respectively. The relation with the first convention is obviously $\tilde{F}(x) = F(x) - D'(x)$. This choice corresponds to the FPE $\partial_t P_t(x) = -\partial_x [\tilde{F}(x) P_t(x)] + \partial_x [D(x) \partial_x P_t(x)]$.

Starting from Itô or Stratonovich SDE : As we have seen in chapter 3, the FPE (4.2) is related to the Itô SDE $dX = F(X) dt + \sqrt{2D(X)} dW(t)$, hence the splitting (4.6) is natural in this case. On the other hand, the Stratonovich SDE $dX = F_S(X) dt + \sqrt{2D(X)} dW(t)$ is related to the FPE $\partial_t P_t(x) = -\partial_x [F_S(x) P_t(x)] + \partial_x (\sqrt{D(x)} \partial_x [\sqrt{D(x)} P_t(x)])$. Thus the current is

$$J_t(x) = F_S(x) P_t(x) - \sqrt{D(x)} \partial_x [\sqrt{D(x)} P_t(x)] \quad \text{where} \quad F_S(x) = F(x) - \frac{1}{2} D'(x) \quad (4.9)$$

cf. Eq. (3.42). This suggests another possible splitting between drift and diffusion contributions (see the discussion in Exercise 3.8). These remarks show that the splitting between drift and diffusion currents is partly arbitrary when $D(x)$ depends on x .

d) Solution for the Fokker-Planck equation in the free case

It is important to have in mind the solution of the FPE in the free case (no drift and uniform diffusion constant). The FPE is then translation invariant, which allows to get a simple solution by using Fourier transformation, in dimension d . We solve $\partial_t P_t(\vec{r}) = D \Delta P_t(\vec{r})$. Introducing

$$\hat{P}_t(\vec{k}) = \int d^d \vec{r} P_t(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} \quad (4.10)$$

we find the first order differential equation

$$\partial_t \hat{P}_t(\vec{k}) = -D \vec{k}^2 \hat{P}_t(\vec{k}) \quad \Rightarrow \quad \hat{P}_t(\vec{k}) = \hat{P}_0(\vec{k}) e^{-D \vec{k}^2 t} \quad (4.11)$$

(Fourier components decouple). For initial condition $P_0(\vec{r}) = \delta(\vec{r} - \vec{r}_0)$ (particle initially at $\vec{r}_0$) we get $\hat{P}_0(\vec{k}) = e^{-i\vec{k} \cdot \vec{r}_0}$, hence $\hat{P}_t(\vec{k}) = e^{-i\vec{k} \cdot \vec{r}_0 - D \vec{k}^2 t}$. Inverse Fourier transform involves a Gaussian integral

$$P_t(\vec{r}) = \int \frac{d^d \vec{k}}{(2\pi)^d} \hat{P}_t(\vec{k}) e^{i\vec{k} \cdot \vec{r}} \quad \Rightarrow \quad P_t(\vec{r}) = \frac{1}{(4\pi Dt)^{d/2}} \exp \left\{ -\frac{(\vec{r} - \vec{r}_0)^2}{4Dt} \right\}. \quad (4.12)$$

The solution is a Gaussian of width $\sim \sqrt{Dt}$ growing in time.

4.2 The generator of the diffusion and the stationary state

The Fokker-Planck equation (4.2) is a linear partial differential equation. For a uniform drift, $D(x) = D$, it can be rewritten as $-\partial_t P_t(x) = H_{\text{FP}} P_t(x)$, where I have introduced the notation $H_{\text{FP}} = -D \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} F(x)$ in order to emphasize the analogy with the Schrödinger equation in imaginary time, whose study usually involves standard methods of spectral analysis.²⁰ With the FPE, a complication however arises due to the fact that the operator $H_{\text{FP}} = -D \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} F(x)$ is *not self-adjoint* in the presence of the drift,²¹ $H_{\text{FP}} \neq H_{\text{FP}}^\dagger$. Let us first make some general remarks on this operator.

a) Generator of the diffusion

Instead of the notation H_{FP} used in [41], I will prefer the mathematicians' notation

$$\partial_t P_t(x) = \mathcal{G}^T P_t(x) \quad \text{where} \quad \mathcal{G}^T = \frac{\partial^2}{\partial x^2} D(x) - \frac{\partial}{\partial x} F(x) \quad (4.13)$$

is the “*adjoint of the generator*” (standard), or the “*forward generator*” (these notes) ; here I have reintroduced a x -dependent diffusion to keep the discussion general (the notation $\mathcal{G}^\dagger$ is also used). By convention, probabilists call the adjoint of this operator

$$\boxed{\mathcal{G} = D(x) \frac{\partial^2}{\partial x^2} + F(x) \frac{\partial}{\partial x}} \quad (4.14)$$

the “*generator of the diffusion*”. I will also call it the “*backward generator*” as we will see that it governs the evolution of the density backward in time. $\mathcal{G}^T$ plays the same role as the matrix of rates W in the master equation (2.31) or the Markov chains' stochastic matrix M in Eq. (2.67) (chapter 2) :

²⁰Here, the notation means that the operator $\frac{\partial}{\partial x} F(x) = F'(x) + F(x) \frac{\partial}{\partial x}$ must be understood as acting on a function $\phi(x)$ as $\frac{\partial}{\partial x} [F(x)\phi(x)] = F'(x)\phi(x) + F(x)\phi'(x)$.

²¹Self-adjointness can be broken not only by the drift term, but also by the boundary conditions if they induce a drift at the boundaries (an example is studied in Exercise ??).

	forward		backward
Markov chains	M	$\leftrightarrow$	M^T
Master equation	W	$\leftrightarrow$	W^T
FPE	$\mathcal{G}^T$	$\leftrightarrow$	$\mathcal{G}$

We have used above that $\left(\frac{\partial}{\partial x}\right)^T = -\frac{\partial}{\partial x}$ (like the adjoint in quantum mechanics, $(\partial_x)^\dagger = -\partial_x$).²²

The generator and its adjoint have interesting structures which can be made more clear after few manipulations. Let us write

$$\frac{\partial^2}{\partial x^2} D(x) - \frac{\partial}{\partial x} F(x) = \frac{\partial}{\partial x} \left(\underbrace{\frac{\partial}{\partial x} - \frac{F(x)}{D(x)}}_{=e^{-U(x)} \frac{\partial}{\partial x} e^{U(x)}} \right) D(x) \quad (4.15)$$

where

$$U(x) \stackrel{\text{def}}{=} - \int^x dx' \frac{F(x')}{D(x')} \quad (4.16)$$

is an “effective potential”. Thus we can rewrite the generator and its adjoint in the following nice forms

$$\mathcal{G}^T = \frac{\partial}{\partial x} e^{-U(x)} \frac{\partial}{\partial x} e^{U(x)} D(x) \quad \text{and} \quad \mathcal{G} = D(x) e^{U(x)} \frac{\partial}{\partial x} e^{-U(x)} \frac{\partial}{\partial x} \quad (4.17)$$

This remark will allow us to obtain straightforwardly the stationary state and will play an important role for the spectral analysis, as we show below.

Case of uniform diffusion : For $D(x) \rightarrow D$, the “effective potential” $U(x) = V(x)/D$ is proportional to the potential energy $V(x) = -\int dx F(x)$. The generator and its adjoint are then

$$\mathcal{G}^T = D \frac{\partial}{\partial x} e^{-V(x)/D} \frac{\partial}{\partial x} e^{V(x)/D} \quad \text{and} \quad \mathcal{G} = D e^{V(x)/D} \frac{\partial}{\partial x} e^{-V(x)/D} \frac{\partial}{\partial x} \quad (4.18)$$

✎ **Exercice 4.1 Form of the generator related to the Stratonovich SDE:** The FPE (4.2) considered above is related to the Itô SDE $dX = F(X) dt + \sqrt{2D(X)} dW(t)$. Instead, we consider here the Stratonovich SDE $dX = F_S(X) dt + \sqrt{2D(X)} dW(t)$.

a) Give the corresponding FPE.

b) Check that the generator has now the more symmetric structure

$$\mathcal{G}^T = \frac{\partial}{\partial x} \sqrt{D(x)} e^{-U_S(x)} \frac{\partial}{\partial x} \sqrt{D(x)} e^{U_S(x)} \quad (4.19)$$

and give the Stratonovich “effective potential” $U_S(x)$. Relate $U_S(x)$ to $U(x)$.

c) Check that the generator and its adjoint are related by a nonunitary transformation of the form $\mathcal{G}^T = \mathcal{U}^{-1} \mathcal{G} \mathcal{U}$.

²²FPE being of the same form as the Schrödinger equation, it involves the same mathematics (spectral analysis for linear differential operators acting in a vector space of functions). In particular, the adjoint of an operator A can be defined from the matrix elements $\langle \Psi^L | A \Phi^R \rangle = \langle A^\dagger \Psi^L | \Phi^R \rangle$, where the scalar product is $\langle \Psi^L | \Phi^R \rangle = \int dx \Psi^L(x) \Phi^R(x)$ (for a real operator $A^\dagger = A^T$). Hence the transposition of ∂_x corresponds to an integration by part, hence the sign.

b) Stationary state

Discussing the master equation, we have noticed that, when a stationary state $P_*(x)$ exists, the convergence of the distribution $P_t(x)$ towards it is exponential (cf. chapter 2 and below). Hence $P_*(x)$ rapidly dominates the properties of the system and for this reason we can often simply focus on the stationary state.

The above remarks on the structure of the generator allow to read off almost directly the stationary state. Let us first recall that in 1D, the stationary current is necessarily a constant : $\partial_t P_t(x) = -\partial_x J_t(x) = 0$ implies that

$$\begin{cases} P_t(x) \rightarrow P_*(x) \\ J_t(x) \rightarrow J \end{cases} \quad (\text{stationarity}).$$

According to the representation (4.17), the probability current related to the stationary state $P_*(x)$ can be conveniently written as

$$J = F(x) P_*(x) - \frac{\partial}{\partial x} [D(x) P_*(x)] = -e^{-U(x)} \frac{\partial}{\partial x} \left[e^{U(x)} D(x) P_*(x) \right]. \quad (4.20)$$

The construction of the stationary state in a finite interval will be discussed in Exercise 4.12. Here, we only discuss the more simple situation where the stationary state is defined on $\mathbb{R}$.

Equilibrium state on $\mathbb{R}$ ($J = 0$).— If the current vanishes, the stationary solution is an equilibrium, which we now denote $P_*(x) \rightarrow P_{\text{eq}}(x)$:

$$P_{\text{eq}}(x) = \frac{c}{D(x)} e^{-U(x)}. \quad (4.21)$$

The condition for equilibrium on $\mathbb{R}$ is the normalisability of this function, $\int_{\mathbb{R}} dx e^{-U(x)} / D(x) < \infty$. This is the case if the potential grows at infinity so that it confines the particle in a certain domain of space. c is a normalisation constant.

Exercise 4.2 : Consider the case $D(x) \rightarrow D$ and discuss precisely the condition on the potential energy $V(x) = -\int dx F(x)$ ensuring the equilibrium. Give an example of a confining potential.

NESS on $\mathbb{R}$ ($J \neq 0$).— When $P_{\text{eq}}(x)$ is not normalisable, the system does not reach equilibrium. Being a second order linear differential equation, $\mathcal{G}^T P(x) = 0$ has two independent solutions. We now search the second solution under the form $P_*(x) = c(x) D(x)^{-1} e^{-U(x)}$ [obtained from $P_{\text{eq}}(x)$ with $c \rightarrow c(x)$]. Introducing the form in (4.20), we deduce that $c'(x) = -J e^{U(x)}$, thus $P_*(x) = -J/D(x) e^{-U(x)} \int^x dy e^{U(y)}$. The lower bound depends on the boundary conditions (this corresponds to choose a constant of integration) : the choice must be consistent with a positive distribution, hence for a diffusion on $\mathbb{R}$ it should be either $-\infty$ or $+\infty$. Now changing the notation as $P_*(x) \rightarrow P_{\text{NESS}}(x)$, we conclude that

$$P_{\text{NESS}}(x) = \frac{J}{D(x)} e^{-U(x)} \int_x^{\pm\infty} dy e^{U(y)}, \quad \text{where } \pm = \text{sign}(J) \quad (4.22)$$

depends whether the potential drives the process from $-\infty$ to $+\infty$ (sign $+$) or the opposite. The condition of existence of the NESS is the normalizability of (4.22). In the case $D(x) \rightarrow D$, we can be more precise : the asymptotic behaviour is obtained by noticing that the drift current is expected to dominate the diffusion current at infinity, see Eq. (4.20), hence $P_{\text{NESS}}(x) \simeq J/F(x)$ for $x \rightarrow \pm\infty$. As a result, the NESS exists if $P_{\text{NESS}}(x)$ is normalisable, which requires $\int_{-\infty}^{\infty} dx/F(x) < \infty$ and $\int_{-\infty}^{+\infty} dx/F(x) < \infty$. Finally, imposing $\int dx P_{\text{NESS}}(x) = 1$ provides a formula for the current J , as a double integral involving $F(x)$ and $D(x)$ (see Exercise 4.15).

We discuss examples with NESS in Exercises 4.11, 4.12 and ??.

Spectral interpretation : The equation for the stationary state has a spectral interpretation : we have identified the right eigenvector for a zero eigenvalue, i.e. $\mathcal{G}^T \Phi_0^R(x) = 0$. Similarly the left eigenvector such that $\mathcal{G} \Phi_0^L(x) = 0$ is clearly a constant :

$$\boxed{\Phi_0^R(x) = P_*(x) \quad \text{and} \quad \Phi_0^L(x) = 1 \quad \text{for e.v. } \lambda_0 = 0} \quad (4.23)$$

where $P_*(x)$ is either $P_{\text{eq}}(x)$ or $P_{\text{NESS}}(x)$. This choice corresponds to the normalisation condition $\int dx \Phi_0^L(x) \Phi_0^R(x) = \int dx P_*(x) = 1$.

We stress again that $P_{\text{eq}}(x)$ and $P_{\text{NESS}}(x)$ are the two independent solutions of $\mathcal{G}^T P(x) = 0$. Only one of the two can be normalised ; if none is normalisable, the process is transient.

Remark (NESS in dimension $d > 1$) : in dimension higher than one, the situation can be much more complicated as stationarity implies $\vec{\nabla} \cdot \vec{J}(\vec{x}) = 0$, hence the NESS may be characterized by a non trivial current distribution $\vec{J}(\vec{x})$.

4.3 Conditional probability, backward FPE and a useful relation

As we emphasized in previous chapters, the propagator of the diffusion (the conditional probability) plays a central role. It is the solution of the FPE for a delta initial condition :

$$\partial_t P_t(x|x_0) = \mathcal{G}_x^T P_t(x|x_0) \quad \text{for } P_0(x|x_0) = \delta(x - x_0), \quad (4.24)$$

where I have now added a label x to make clear that the differential operator acts on the coordinate x (and not x_0). As pointed out earlier, the FPE involves the same mathematics as the Schrödinger equation, hence it is tempting to use similar notations and write the solution of (4.24) as

$$\boxed{P_t(x|x_0) = \langle x | e^{t\mathcal{G}^T} | x_0 \rangle} \quad (4.25)$$

where $|x_0\rangle$ represents the state (distribution) for a particle at (initial) position x_0 and $e^{t\mathcal{G}^T}$ is the evolution operator for the distribution.

a) Forward and backward FPE

Preliminary : transposition of the master equation.— FPE is a specific form of the master equation, thus the analogy with the master equation (2.31) for discrete states is a good starting point. We have obtained the expression of the conditional probability : $P_t(n|m) = (e^{tW})_{nm} = (e^{tW^T})_{mn}$. Here, the correspondence is $W \rightarrow \mathcal{G}^T$ and $W^T \rightarrow \mathcal{G}$. Writing that $\partial_t e^{tW} = W e^{tW}$ gives the “forward master equation”

$$\partial_t P_t(n|n_0) = \sum_m W_{nm} P_t(m|n_0) \quad (4.26)$$

whereas starting from $\partial_t e^{tW} = e^{tW} W$, we get the “backward master equation”

$$\partial_t P_t(n|n_0) = \sum_m (W^T)_{n_0 m} P_t(n|m). \quad (4.27)$$

Application to the FPE.— The representation (4.25) is the continuous version of (2.65) [or (2.78)], and the FPE (4.24) corresponds to (4.26). Let us now discuss the continuous version of (4.27). The transposition of the propagator is $P_t(x|x_0) = \langle x_0 | e^{t\mathcal{G}} | x \rangle$,²³ hence we have

$$\partial_t P_t(x|x_0) = \partial_t \langle x_0 | e^{t\mathcal{G}} | x \rangle = \mathcal{G}_{x_0} \langle x_0 | e^{t\mathcal{G}} | x \rangle = \mathcal{G}_{x_0} P_t(x|x_0)$$

²³In quantum mechanics, one writes $\langle \psi | A^\dagger | \chi \rangle = \langle \psi | A^\dagger | \chi \rangle = \langle \chi | A | \psi \rangle^* = \langle \chi | A \psi \rangle^*$. In the text, the matrix element is real.

Let us now summarize the two important forms of FPE obtained. We call the first form the “*forward FPE*”

$$\boxed{\partial_t P_t(x|x_0) = \mathcal{G}_x^T P_t(x|x_0)} \quad \text{for } \mathcal{G}_x^T = \partial_x^2 D(x) - \partial_x F(x) \quad (4.28)$$

where the forward generator acts on the *final* coordinate x . The operator $\mathcal{G}_x^T$ controls the evolution *forward* in time.

Then, we have obtained a second equivalent form

$$\boxed{\partial_t P_t(x|x_0) = \mathcal{G}_{x_0} P_t(x|x_0)} \quad \text{for } \mathcal{G}_x = D(x) \partial_x^2 + F(x) \partial_x \quad (4.29)$$

where the operator acts on the *initial* coordinate x_0 , i.e. controls the evolution *backward* in time (in the past). For this reason, (4.29) is called the “*backward FPE*”. We will see some applications of this equation below.

Remark : The above discussion can be reformulated as follows : $\partial_t P_t(x|x_0) = \langle x | \mathcal{G}^T e^{t\mathcal{G}^T} | x_0 \rangle = \mathcal{G}_x^T \langle x | e^{t\mathcal{G}^T} | x_0 \rangle$ and equivalently $\partial_t P_t(x|x_0) = \langle x | e^{t\mathcal{G}^T} \mathcal{G}^T | x_0 \rangle = \mathcal{G}_{x_0} \langle x | e^{t\mathcal{G}^T} | x_0 \rangle$.

b) A useful identity

The nice representation (4.17) can be rewritten

$$\mathcal{G}^T = \frac{\partial}{\partial x} D(x) P_{\text{eq}}(x) \frac{\partial}{\partial x} P_{\text{eq}}(x)^{-1} \quad (4.30)$$

where $P_{\text{eq}}(x) = D(x)^{-1} e^{-U(x)}$. This shows that the generator and its adjoint are related by the non-unitary transformation

$$\boxed{P_{\text{eq}}(x)^{-1} \mathcal{G}^T P_{\text{eq}}(x) = \mathcal{G}} \quad (4.31)$$

We stress that here, we do NOT assume that the equilibrium exists. If $\int dx P_{\text{eq}}(x) < \infty$, then the process reaches an equilibrium, however the discussion also applies to the case $\int dx P_{\text{eq}}(x) = \infty$ (NESS or transient process).

We have shown above that $P_t(x|x_0) = \langle x | e^{t\mathcal{G}^T} | x_0 \rangle = \langle x_0 | e^{t\mathcal{G}} | x \rangle$. If we combine this with (4.31), the r.h.s. rewrites

$$\langle x_0 | e^{t\mathcal{G}} | x \rangle = \langle x_0 | P_{\text{eq}}(x)^{-1} e^{t\mathcal{G}^T} P_{\text{eq}}(x) | x \rangle = \frac{P_{\text{eq}}(x)}{P_{\text{eq}}(x_0)} \langle x_0 | e^{t\mathcal{G}^T} | x \rangle \quad (4.32)$$

i.e. we have obtained the following relation

$$\boxed{P_t(x|x_0) P_{\text{eq}}(x_0) = P_t(x_0|x) P_{\text{eq}}(x)} \quad \text{where } P_{\text{eq}}(x) = e^{-U(x)} / D(x). \quad (4.33)$$

Eq. (4.33) is interesting as it allows to exchange the role of the two coordinates of the conditional probability. We emphasize again that it does NOT require $P_{\text{eq}}(x)$ to be normalisable. Hence, $P_{\text{eq}}(x)$ can not always be interpreted here as a distribution.

🔪 **Exercice 4.3 BFPE from FFPE :** Deduce (4.29) from (4.28) by using (4.33).

The specific case of processes with an equilibrium.— Let us now assume that $P_{\text{eq}}(x)$ is normalisable and discuss some consequences of this additional assumption. We first point out that although the relation is reminiscent of the detailed balance condition, it should not be confused with it. The detailed balance condition involves the transition rates, i.e. the $t \rightarrow 0$ limit of the relation (4.33) : $P_t(x|x_0) \simeq \delta(x - x_0) + t W(x|x_0)$, then

$$W(x|x_0)P_{\text{eq}}(x_0) = W(x_0|x)P_{\text{eq}}(x) \quad (\text{detailed balance}), \quad (4.34)$$

which only holds when there is an equilibrium, i.e. $P_{\text{eq}}(x)$ is normalisable, whereas (4.33) is completely general.

When $P_{\text{eq}}(x)$ is normalisable, we can also interpret (4.33) as a representation of the two point function : from the definition of the conditional probability (chapter 2) $P_2(x, t; x_0, 0) = P_t(x|x_0)P_{\text{eq}}(x_0)$, so that (4.33) is

$$P_2(x, t; x_0, 0) = P_2(x_0, t; x, 0). \quad (4.35)$$

If we combine the relation with time translation invariance, we get

$$P_2(x, t; x_0, 0) = P_2(x_0, 0; x, -t). \quad (4.36)$$

The probability to be at x and x_0 at two different times is independent of the direction in which the particle is going (from x_0 to x or from x to x_0). This equation reveals some *time reversal invariance*, reminiscent of the micro-reversibility encoded in detailed balance.

4.4 Relaxation and spectral analysis

The spectral analysis already presented for the master equation (chapter 2, § 2.5) has shown that when the stationary state (equilibrium or NESS) exists, it appears as an isolated zero mode of the underlying linear operator. This is also true for the FPE (there is a finite gap between $\lambda_0 = 0$ and the eigenvalues of the excited eigenvectors, unless the process is transient). The convergence of the time dependent solution $P_t(x)$ towards the stationary state is therefore *exponentially* fast. This means that the stationary state rapidly dominates the physics. On the other hand, the full spectral information provides details on the dynamics on short time scale and how the system reaches equilibrium or stationary state, allowing to identify a relaxation time.²⁴

When the process is transient (no stationary state), the full time dependent analysis is crucial.

a) Solving the FPE

Let us apply the spectral method to solve the FPE $\partial_t P_t(x) = \mathcal{G}^T P_t(x)$. When the operator is time independent, $F(x, t) \rightarrow F(x)$ and $D(x, t) \rightarrow D(x)$, we can look for a solution under the “separable” form

$$P_t(x) = \Phi(x) e^{-\lambda t} \quad \text{hence} \quad \mathcal{G}^T \Phi(x) = -\lambda \Phi(x). \quad (4.37)$$

Because the generator is not self adjoint, this last equation is an equation for a “right eigenvector” of $\mathcal{G}^T$. Its spectrum involves a bi-orthogonal set of right and left eigenvectors

$$\mathcal{G}^T \Phi_n^R(x) = -\lambda_n \Phi_n^R(x) \quad \text{and} \quad \mathcal{G} \Phi_n^L(x) = -\lambda_n \Phi_n^L(x) \quad (4.38)$$

²⁴In quantum mechanics, the situation is completely different. The Schrödinger equation $i\hbar \partial_t \Psi(x, t) = H \Psi(x, t)$ being complex, at any time in the future the dynamics involves all eigenstates which are initially occupied with finite probability : $\Psi(x, t) = \sum_n c_n e^{-iE_n t/\hbar} \psi_n(x)$, where $H \psi_n(x) = E_n \psi_n(x)$. Unless there is a reason to fall into the ground state (dissipation), the ground state does not dominate the dynamics in general. The full spectral information is essential in QM.

We now discuss the orthonormalisation condition. Let us multiply $\mathcal{G}^T \Phi_n^R(x) = -\lambda_n \Phi_n^R(x)$ by $\Phi_m^L(x)$ and $\mathcal{G} \Phi_m^L(x) = -\lambda_m \Phi_m^L(x)$ by $\Phi_n^R(x)$. After integration, the difference is

$$\int dx [\Phi_m^L(x) \mathcal{G}^T \Phi_n^R(x) - \Phi_n^R(x) \mathcal{G} \Phi_m^L(x)] = (\lambda_n - \lambda_m) \int dx \Phi_m^L(x) \Phi_n^R(x). \quad (4.39)$$

The l.h.s. is zero by using the definition of transposition, hence $\int dx \Phi_m^L(x) \Phi_n^R(x) = 0$ for $\lambda_n \neq \lambda_m$. A convenient choice of normalisation is

$$\int dx \Phi_n^L(x) \Phi_n^R(x) = \delta_{n,m} \quad (4.40)$$

(see the discrete version in Subsection 2.5 page 30). Note that this requires that $\Phi_n^L(x) \Phi_n^R(x)$ decays sufficiently fast at infinity (we will see on an example that the left eigenfunction may grows at infinity, which is not a problem provided that the right eigenfunction decays fast enough).

We now use the spectral information to solve the FPE for a given initial condition $P_0(x)$. We first decompose this latter on the right eigenvectors

$$P_0(x) = \sum_n c_n \Phi_n^R(x) \quad \text{where} \quad c_n = \int dx \Phi_n^L(x) P_0(x) \quad (4.41)$$

Then, the solution at time t reads

$$P_t(x) = \sum_n c_n \Phi_n^R(x) e^{-\lambda_n t}. \quad (4.42)$$

Because $\Phi_0^L(x) = 1$, the $n = 0$ term for e.v. $\lambda_0 = 0$ carries all the normalisation of the solution, $c_0 = \int dx P_t(x) = 1$, hence

$$P_t(x) = \Phi_0^R(x) + \sum_{n(\neq 0)} c_n \Phi_n^R(x) e^{-\lambda_n t} \simeq P_*(x) + \mathcal{O}(e^{-t/\tau_{\text{relax}}}) \quad (4.43)$$

where the eigenvalue λ_1 corresponds to the lowest *relaxation rate* $1/\tau_{\text{relax}} = \lambda_1$ (or $\text{Re}(\lambda_1)$ if λ_1 is complex). When there exists an *equilibrium*, for a confining potential $V(x)$, the spectrum is real as we will argue below.

We have described the situation where the lowest eigenvalue $\lambda_0 = 0$ is isolated (there is a finite gap between λ_0 and the next eigenvalue), when there exists a stationary state $P_* \rightarrow P_{\text{eq}}$ or P_{NESS} . In the case of transient process, the spectrum of eigenvalues is continuous and the large time properties are not dominated by a single eigenvalue (see Exercise ??).

Spectral decomposition of the conditional probability (propagator).— The conditional probability is the solution of the (forward) FPE for the initial condition $P_t(x|x_0)|_{t=0} = \delta(x-x_0)$. We deduce the coefficient in (4.42) from the initial condition $c_n = \int dx \Phi_n^L(x) P_0(x|x_0) = \Phi_n^L(x_0)$. Therefore the spectral decomposition of the conditional probability is

$$\boxed{P_t(x|x_0) = \sum_n \Phi_n^R(x) \Phi_n^L(x_0) e^{-\lambda_n t}} \quad (4.44)$$

It may also be useful to give a more formal representation of the propagator : the orthonormalisation condition (4.40) implies the dual relation $\sum_n \Phi_n^R(x) \Phi_n^L(x') = \delta(x-x')$, or more formally $\sum_n |\Phi_n^R\rangle \langle \Phi_n^L| = 1$. As a result we can rewrite (4.44) as $P_t(x|x_0) = \langle x | (\sum_n |\Phi_n^R\rangle \langle \Phi_n^L| e^{-\lambda_n t}) | x_0 \rangle$, where inside the paranthesis is the spectral representation of the operator $e^{t\mathcal{G}^T}$, cf. Eq. (4.25).

Devil is in the details.— Eigenfunctions can be found by solving (4.38), however we have eluded the important question of boundary conditions. In principle, a spectral problem requires to specify boundary conditions (at infinity if the diffusion is defined on $\mathbb{R}$). We first discuss the case of confining drift, when the discussion is more simple, and will only make few remarks on the more subtle case of NESS at the end of the subsection.

4.5 Boundary conditions for the FPE

So far we have not discussed the situation where the FPE is solved on a bounded domain. Let us discuss here the question of boundary conditions. For simplicity we consider the FPE for a uniform diffusion constant $\partial_t P_t(x) = [D\partial_x^2 - \partial_x F(x)]P_t(x) = -\partial_x J_t(x)$ on $\mathbb{R}^+$ so that there is just one boundary at $x = 0$.

a) Reflecting boundary condition

The first natural boundary condition is the reflecting boundary condition : the particle arriving at the origin $x = 0$ is simply reflected and remains in $\mathbb{R}^+$. This is expressed by the condition of a vanishing current at the origin

$$J_t(0) = F(0)P_t(0) - DP_t'(0) = 0 \quad (4.45)$$

where ' means here derivation with respect to x . In the usual terminology, this corresponds to a “mixed boundary condition”.²⁵

Remark : reflecting boundary conditions for the conditional probability.— For the following we will have to impose the boundary conditions on the conditional probability $P_t(x|x_0)$. The reflecting boundary condition is a *mixed* boundary condition

$$[D\partial_x - F(x)]P_t(x|x_0)|_{x=0} = 0 \quad (4.46)$$

We could also ask about the condition with respect to the initial coordinate : using the relation (4.33), we have

$$\left(\partial_x - \frac{1}{D}F(x)\right)P_t(x|x_0) = \left(\partial_x + \frac{1}{D}V'(x)\right)\left[\frac{P_{\text{eq}}(x)}{P_{\text{eq}}(x_0)}P_t(x_0|x)\right] = \frac{P_{\text{eq}}(x)}{P_{\text{eq}}(x_0)}\partial_x P_t(x_0|x) \quad (4.47)$$

where I have used that $P_{\text{eq}}(x) \propto \exp[-V(x)/D]$. As a consequence, the presence of the reflecting boundary implies a *Neumann* boundary condition with respect to the variable x_0 :

$$\partial_{x_0}P_t(x|x_0)|_{x_0=0} = 0. \quad (4.48)$$

The reflecting boundary condition is not symmetric with respect to the two coordinates.

²⁵For a linear wave equation of second order for the wave $\psi(x)$, like the Schrödinger equation $-\psi''(x) + V(x)\psi(x) = E\psi(x)$, the standard terminology is :

(i) **Dirichlet** boundary condition : $\psi(0) = 0$;
(ii) **Neumann** boundary condition : $\psi'(0) = 0$;
(iii) **mixed** boundary condition : $\psi(0)\cos\theta + \psi'(0)\sin\theta = 0$ (one recovers Dirichlet and Neumann b.c. for $\theta = 0$ and $\theta = \pi/2$, respectively).

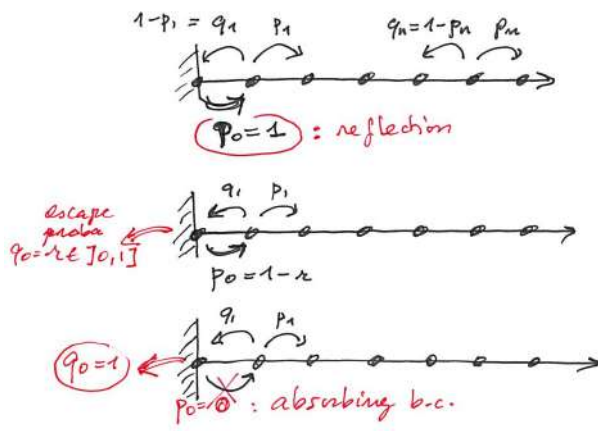


Figure 4.3: The different choices of boundary conditions are illustrated by considering a discrete random walk on the semi-infinite line (Markov chain). The particle at site n jumps to the right with probability $p_n \in [0, 1]$ or to the left with probability $q_n = 1 - p_n$. The different boundary conditions correspond to different choices for the probability p_0 , given that the particle leaving the semi-infinite axis to the left with probability $q_0 = r \in]0, 1]$ does not come back : reflecting b.c. (top), general b.c. (middle) and absorbing b.c. (bottom).

b) General boundary condition

Since the Fokker-Planck generator is a second order differential operator, the most general boundary condition involve a linear combination of $P(0)$ and $P'(0)$ at the boundary $x = 0$. Let us now consider a general (mixed) boundary condition

$$\tilde{\lambda} P_t(0) = P'_t(0) . \quad (4.49)$$

For $\tilde{\lambda} = F(0)/D$, this corresponds to the reflecting boundary condition. What is the meaning of this condition for arbitrary real $\tilde{\lambda} \neq F(0)/D$?

Consider

$$\partial_t \int_0^\infty dx P_t(x) = - \int_0^\infty dx \partial_x J_t(x) = J_t(0) \quad (4.50)$$

The current of probability through $x = 0$ makes the total probability decrease (for $J_t(0) < 0$). Making use of the boundary condition, we get

$$J_t(0) = [F(0) - D\tilde{\lambda}] P_t(0) \equiv -\lambda P_t(0) \quad (4.51)$$

where we have found convenient to introduce $\lambda = D\tilde{\lambda} - F(0)$. For $\lambda > 0$, the total probability decreases

$$\partial_t \int_0^\infty dx P_t(x) = -\lambda P_t(0) . \quad (4.52)$$

Hence $\lambda > 0$ has roughly the meaning of the rate of escape when the particle is at the boundary $x = 0$. Being at $x = 0$, the particle is absorbed ("killed") or reflected with finite probabilities. The total probability $\int_0^\infty dx P_t(x)$ decreases with time because the particle touching the boundary is absorbed, i.e. leaves the system.

c) Absorbing boundary condition

Writing $P_t(0) = \tilde{\lambda}^{-1} P'_t(0)$ shows that the limit $\tilde{\lambda} \rightarrow \infty$, or $\lambda \rightarrow \infty$, corresponds to a Dirichlet boundary condition

$$P_t(0) = 0 \quad (4.53)$$

describing physically the situation where the particle reaching the boundary is absorbed with probability one (like the mouse on Fig. 4.4).

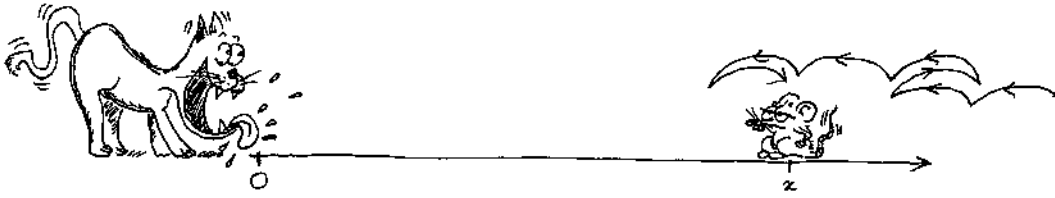


Figure 4.4: A random walker (the mouse) with an absorbing boundary condition at $x = 0$ (the cat).

d) Periodic boundary conditions

Consider the interval $[0, L]$. For periodic boundary conditions (i.e. a ring) the physical quantities like the density and the current should be continuous :

$$P_t(0) = P_t(L) \quad \text{and} \quad J_t(0) = J_t(L) \quad (4.54)$$

Examples are discussed in the following exercise and in Exercise 4.12.

Exercise 4.4 The pendulum in the overdamped regime: We consider a pendulum in a fluid, in the overdamped regime, described by the Fokker-Planck equation

$$\partial_t P_t(\theta) = D \partial_\theta^2 P_t(\theta) - \partial_\theta [(v - k \sin \theta) P_t(\theta)] \quad \text{for } \theta \in [-\pi, +\pi] \quad (4.55)$$

a) Relate the drift to a potential $U(\theta)$ and show that, for $v = 0$, the FPE admits an equilibrium state $P_{\text{eq}}(\theta)$.

b) Argue that this solution is not satisfactory and that there is no equilibrium when $v \neq 0$.

c) To simplify the calculation, we set $D = 1$. Show that the stationary state has the form

$$P_{\text{NESS}}(\theta) = J \psi(\theta) \left[c + \int_\theta^\pi \frac{d\alpha}{\psi(\alpha)} \right] \quad \text{where } \psi(\theta) = e^{-U(\theta)}. \quad (4.56)$$

Find c . What is the physical meaning of J ? Is it a free parameter ? Express J .

d) Analyze the limiting behaviour of J when $v \rightarrow 0$; use the modified Bessel function $I_0(z) = \int_0^{2\pi} \frac{dt}{2\pi} e^{z \cos t}$ (see Appendix A for its asymptotic behaviour).

4.6 First passage and exit problem (in 1D)

We now study the recurrence for general diffusions in one-dimension (the restriction to dimension one makes the calculations simple ; the method extends easily to dimensions $d > 1$).

a) Persistence of the free Brownian motion

Here, I come back to the problem studied in § ?? : we study (in Exercise 4.5) the question of the first return of the free Brownian motion. In the previous paragraph, we considered the same question for the discrete random walk ; here we reconsider the problem for a continuous Brownian motion. This is the “*persistence*” problem, as the first return probability at time t corresponds to the probability that the process “persists” to remain positive up to time t .

Exercise 4.5 Persistence, first passage time and maximum of the BM:

a) **Propagator on the half line.**— We consider the free diffusion on $\mathbb{R}_+$ with a Dirichlet boundary condition at the origin. Construct the solution of the diffusion equation

$$\partial_t P_t(x) = D \partial_x^2 P_t(x) \quad \text{for } x > 0 \text{ with } P_t(0) = 0 \quad (4.57)$$

(use the image method). Apply the method to get the propagator of the diffusion on $\mathbb{R}_+$, denoted $P_t^{(\text{Dir})}(x|x_0)$.

b) **Survival probability.**— Dirichlet boundary condition describes absorption at $x = 0$. Compute the survival probability for a particle starting from x_0 :

$$S_{x_0}(t) = \int_0^\infty dx P_t^{(\text{Dir})}(x|x_0) \quad (4.58)$$

What would have been the result for $P_t^{(\text{Neu})}(x|x_0)$, the solution for a Neumann boundary condition, $\partial_x P_t(x)|_{x=0} = 0$?

c) **First passage time.**— We denote by T_{x_0} the first time at which the process starting from $x_0 > 0$ reaches $x = 0$ (it is a random quantity depending on the process), and $\mathcal{P}_{x_0}(T)$ its distribution. Deduce

$$\mathcal{P}_{x_0}(T) = \frac{x_0}{\sqrt{4\pi D} T^{3/2}} e^{-\frac{x_0^2}{4DT}}. \quad (4.59)$$

Plot neatly the distribution and compare with the result obtained for the RW on the lattice.

d) **Maximum of a BM.**— We now consider another property of the Brownian motion $x(\tau)$ with $\tau \in [0, t]$ starting from $x_0 = 0$: we denote by $M = \max_{\tau \in [0, t]} (x(\tau)) \geq 0$ its maximum and $W_t(m)$

the distribution of M . Show that $W_t(m)$ and $S_{x_0}(t)$ are related and deduce the expression of $W_t(m)$. What does $W_t(0)$ represent ? The exponent of the power law $t^{-\theta}$ is called the persistence exponent. Give θ for the Brownian motion.

Hint : use Appendix A with properties of the error function.

Remark : we have recovered the results obtained within the discrete model of random walk (§ ??) : the probability to return to the starting point is $P_t(0|0) \sim t^{-1/2}$ and the probability for the first return is $\mathcal{P}_{x_0}(t) \sim t^{-3/2}$ at large time.

Conclusion of this analysis.— we can already make two important remarks :

- the study of a first passage time problem requires to *impose an absorbing boundary condition at the target point*, here $x = 0$.
- The definition of the survival probability suggests that one should first find the conditional probability, then integrate it to get the survival probability. In fact, the *backward FPE* provides a shortcut and allows to find an equation directly for the survival probability, as we will see.

b) First passage time for arbitrary drift

We consider the case of a diffusion with drift and uniform diffusion constant for simplicity

$$dX(t) = F(X) dt + \sqrt{2D} dW(t) \quad (4.60)$$

The drift derives from a potential $F(x) = -V'(x)$ and $W(t)$ is the Wiener process. Consider that the diffusion starts from the initial condition $x(0) = x_0$.

The determination of the propagator $P_t(b|x_0)$ allows to answer the question : what is the probability that the process reaches the point $x = b$ in a (fixed) time t (i.e. the final position is the random variable). We now ask a dual question : *what is the time T_{x_0} needed to reach the point $x = b$ for the first time ?* We consider trajectories such that :

$$\begin{cases} x(0) = x_0 \\ x(t) < b \text{ for } 0 < t < T_{x_0} \\ x(T_{x_0}) = b. \end{cases} \quad (4.61)$$

Hence we now fix the final position ($x = b$) and study the statistical properties of the random time T_{x_0} . We denote by $\mathcal{P}_{x_0}(T)$ its distribution.

The main idea is to introduce an **absorbing boundary** at the target point :

$$\boxed{P_t(b|x_0) = P_t(x|b) = 0} \quad (4.62)$$

implying that the particle is absorbed when it reaches $x = b$ (cf. Fig. 4.4). This condition implies that the calculations will exclude all trajectories passing through $x = b$. For simplicity for future calculations and analysis, we also impose a *reflecting boundary condition* at another point $x = a < b$, i.e. we impose that the current vanishes

$$(F(x) - D\partial_x) P_t(x|x_0)|_{x=a} = \partial_{x_0} P_t(x|x_0)|_{x_0=a} = 0 \quad (4.63)$$

The boundary condition takes a different form with respect to the two arguments (this is expected as $P_t(x|x_0)$ is not a symmetric function of its two arguments in general, cf. § 4.5 page 66).

We introduce the **survival probability**

$$S_{x_0}(t) = \text{Proba}\{x(\tau) < b \text{ for } \tau \in [0, t]\} = \int_a^b dx P_t(x|x_0), \quad (4.64)$$

the probability that the particle has survived up to time t , i.e. has not reached the absorbing boundary at $x = b$. Due to the absorbing boundary, $S_{x_0}(t) \leq 1$. The survival probability is also the probability for the particle to be absorbed after time t

$$S_{x_0}(t) = \text{Proba}\{T_{x_0} \geq t\} = \int_t^\infty dT \mathcal{P}_{x_0}(T). \quad (4.65)$$

Then $\mathcal{P}_{x_0}(T) = -\partial_T S_{x_0}(T)$. Because we integrate over the final position x of the propagator, the forward FPE is not helpful. Instead, making use of the *backward* FPE (4.29) allows to obtain a PDE for the survival probability

$$\partial_t S_{x_0}(t) = \int_a^b dx \mathcal{G}_{x_0} P_t(x|x_0) = \mathcal{G}_{x_0} S_{x_0}(t), \quad (4.66)$$

where the PDE is solved for the initial condition

$$S_{x_0}(0) = \begin{cases} 1 & \text{for } x_0 \in [a, b[\\ 0 & \text{for } x_0 \geq b \end{cases}. \quad (4.67)$$

Similarly the first passage time distribution obeys

$$\partial_t \mathcal{P}_{x_0}(t) = \mathcal{G}_{x_0} \mathcal{P}_{x_0}(t) \quad (4.68)$$

At this point it is useful to introduce the n -th moment of the time :

$$T_n(x_0) \stackrel{\text{def}}{=} \langle (T_{x_0})^n \rangle = \int_0^\infty dT T^n \mathcal{P}_{x_0}(T) \quad (4.69)$$

✎ Exercise 4.6 Moments of the first passage time :

a) Show that the moments obey the recurrence

$$\mathcal{G}_{x_0} T_n(x_0) = -n T_{n-1}(x_0) \quad \text{and} \quad \mathcal{G}_{x_0} T_1(x_0) = -1. \quad (4.70)$$

b) Justify that the boundary conditions are $\partial_{x_0} T_n(x_0)|_{x_0=a} = 0$ and $T_n(b) = 0$.

c) Deduce (calculation requires to solve a first order linear differential equation: easy!)

$$\boxed{T_n(x_0) = \frac{n}{D} \int_{x_0}^b dx e^{V(x)/D} \int_a^x dx' e^{-V(x')/D} T_{n-1}(x')} \quad (4.71)$$

(with obviously $T_0(x_0) = 1$).

c) Lifetime of a metastable state (Arrhenius law)

An important application of the above formalism is the analysis of the escape time for a particle trapped in a potential well. This problem is relevant in chemistry where chemical reactions are activated by overcoming some potential (activation) barriers in the configuration space of the molecules. For simplicity we consider a one-dimensional problem of a particle initially in a potential well (Fig. 4.5) : x_0 is close to the local minimum at x_1 . We study the time needed to escape the well, i.e. jump in the region $x > x_2$.

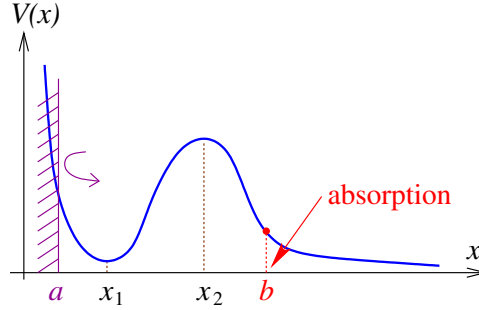


Figure 4.5: A particle escapes from a metastable state.

In a rather arbitrary manner, we introduce a reflecting boundary at $x = a$ at the left of the local minimum, and the absorbing boundary at $x = b$ at the right of the potential barrier (not too close from the top). As we have seen above the average time is given by

$$T_1(x_0) = \frac{1}{D} \int_{x_0}^b dx e^{V(x)/D} \int_a^x dx' e^{-V(x')/D}. \quad (4.72)$$

The integral can be analysed by using the steepest descent method. For $D \rightarrow 0$, the integral over x is dominated by the neighbourhood of $x = x_2$, hence we can replace the upper bound of the second integral $\int_a^x \rightarrow \int_a^{x_2}$, expand the potential in the exponential $e^{V(x)/D} \simeq \exp \left\{ \frac{1}{D} [V(x_2) - \frac{1}{\delta_2^2} (x - x_2)^2] \right\}$, where $\delta_2 = 1/\sqrt{-V''(x_2)}$, and perform the remaining Gaussian integral. Similarly, the integral over x' is dominated by the neighbourhood of $x' = x_1$; expanding similarly the integrand as $e^{-V(x')/D} \simeq \exp \left\{ \frac{1}{D} [-V(x_1) - \frac{1}{\delta_1^2} (x' - x_1)^2] \right\}$, where $\delta_1 = 1/\sqrt{V''(x_1)}$, we end with

$$\langle T_{x_0} \rangle \equiv T_1(x_0) \simeq 2\pi \delta_1 \delta_2 \exp \left\{ \frac{V(x_2) - V(x_1)}{D} \right\} \quad (4.73)$$

The main result is that the average time is exponentially large in the height of the potential barrier $\Delta V = V(x_2) - V(x_1)$. It is pretty independent of x_0 (provided that it remains in the well) : for x_0 in the well, the particle is rapidly driven at the bottom of the well, where it is submitted to the fluctuations (the time scale is controlled by the curvature at x_1 , like for the Ornstein-Uhlenbeck process) ; then it takes a long time to escape the well, thanks to a large (and thus rare) thermal fluctuation.

A remark (dimensional analysis) : as physicists, it is always good to remember dimensional analysis. Here, the SDE (4.60) describes the overdamped regime for a particle in the force field $F(x)$, hence we include the friction coefficient γ in the force. As a result the “potential” $V(x) = E_{\text{pot}}(x)/\gamma$ has dimension $E/[\gamma] = (ML^2T^{-2})/(MT^{-1}) = L^2T^{-1}$, i.e. has the same dimension as the diffusion constant $[D] = L^2T^{-1}$, as it should since the combination $V(x)/D$ appears in exponentials and should be dimensionless. For this reason, the curvatures $\delta_{1,2}^2$ have the dimension of a time.



Figure 4.6: The Swedish chemist Svante August Arrhenius (1859-1927), Nobel prize in chemistry in 1903.

✎ **Exercise 4.7 :** How far from the top of the barrier (at x_2) must be the absorbing boundary b so that the previous analysis is justified ? And how far the reflecting boundary at a should be from the bottom of the well (at x_1) ?

✎ **Exercise 4.8 Time needed to fall at the bottom of a harmonic well:** We discuss the situation where the initial point x_0 is far from the minimum of the well at $x = x_1$ and clarify a point of the previous discussion. We consider the Ornstein-Uhlenbeck process $\frac{d}{dt}x(t) = -\lambda(x - x_1) + \sqrt{2D}\eta(t)$. What is the typical time needed by a particle initially far from the minimum, $x(0) - x_1 = \Delta$ “large”, to fall in the potential well ? Compare to the Arrhenius time.

We can also analyze higher moments : applying the same arguments to (4.71) we get

$$T_n(x_0) \simeq n T_{n-1}(x_1) T_1(x_0) \quad (4.74)$$

for $D \rightarrow 0$. Using the independence in the initial position, we conclude that the moments are

$$T_n(x_0) \simeq n! [T_1(x_0)]^n \quad (4.75)$$

i.e. those of a Poisson distribution.

$$\boxed{\mathcal{P}_{x_0}(T) \simeq \frac{1}{\langle T_{x_0} \rangle} \exp \left\{ -\frac{T}{\langle T_{x_0} \rangle} \right\}} \quad (4.76)$$

The exponential distribution was expected as in the $D \rightarrow 0$ limit, the particle is trapped a long time in the well, hence has time to decorrelate : the picture is that, starting from the initial position x_0 , the particle falls after a short time in the vicinity of the minimum of the potential well $x(t) \sim x_1$. There, fluctuations are $\delta x \sim \sqrt{D}/\delta_1$. As long as the process remains in the well, it is approximatively described by the Langevin equation $\frac{d}{dt}x(t) \approx -\frac{1}{\delta_1^2}(x - x_1) + \sqrt{2D}\eta(t)$, where we have linearized $F(x) = -V'(x)$ near x_1 . The correlation function is $\langle x(t)x(t') \rangle_c \simeq (D/\delta_1^2) \exp[-|t - t'|/\delta_1^2]$ (cf. chapter 1 on Langevin equation). Indeed, the decorrelation time is $\sim \delta_1^2$, which is exponentially smaller than the typical time needed to escape the well. This shows that the escape process can be approximatively considered Markovian, hence the exponential distribution (4.76).

☺ Important points

- Have in mind the meaning of the two terms in the FPE (drift and diffusion).
- Conservation equation $\partial_t P = -\partial_x J$ (or $\partial_t P = -\vec{\nabla} \cdot \vec{J}$ in $d > 1$) and recover the expression of the current.

- Remember the solution of the FPE in the free case, $\partial_t P = D \Delta P$ (in dimension d), or be able to recover it in two lines by Fourier transform in space :
 $P_t(\vec{r}|\vec{r}_0) = (4\pi Dt)^{-d/2} \exp\left\{-\frac{(\vec{r}-\vec{r}_0)^2}{4Dt}\right\}$
- Existence of the BFPE
- Be familiar with the different types of boundary conditions (reflecting, absorbing)
- The problem of first passage time (relation between survival probability and the distribution of the first passage time) ; the use of the BFPE.
- Study of the first passage at point $x = b$ requires to consider an absorbing boundary at this place and determine the “survival probability”.
- The Arrhenius law.

Additional exercises

✎ **Exercise 4.9 FPE for a linear drift:** We study a diffusion on $\mathbb{R}$ for a linear drift, described by the Fokker-Planck equation

$$\partial_t P_t(x) = -\partial_x[(a + bx)P_t(x)] + \partial_x^2[D(x)P_t(x)] . \quad (4.77)$$

- 1/ Express $\frac{d}{dt}\langle X(t) \rangle$ in terms of $P_t(x)$. Deduce that $\langle X(t) \rangle$ obeys a simple differential equation. Solve this differential equation for initial condition $X(0) = 0$. Discuss the solution briefly : assuming $a > 0$, plot neatly $\langle X(t) \rangle$ for $b > 0$ and $b < 0$.
- 2/ Consider now $\frac{d}{dt}\langle X(t)^n \rangle$. Under what condition on $D(x)$ would it be possible in principle to solve a differential equation for $\langle X(t)^n \rangle$? (do not solve it yet).
- 3/ We choose $D(x) = D_0 + D_1 x + D_2 x^2$ ($> 0 \forall x$). Show that the variance $\langle X(t)^2 \rangle_c = \langle X(t)^2 \rangle - \langle X(t) \rangle^2$ obeys a linear differential equation with a source term $D(\langle X(t) \rangle)$. Solve the equation for $x(0) = 0$. Estimate the main behaviour for large t (for $b > 0$ and $D_2 > 0$). Discuss $\sqrt{\langle X(t)^2 \rangle_c} / \langle X(t) \rangle$ in this limit.

✎ **Exercise 4.10 FPE without drift and for x -dependent diffusion constant:** We consider the Stratonovich SDE $dX(t) = \sqrt{2D(X)} dW(t)$, for $D(x) > 0 \forall x \in \mathbb{R}$. The aim is to discuss the large time behaviour of the solution of the FPE.

a) Write the FPE for $P_t(x)$. Can a steady state exist ?

Assuming $D(x) = D(-x)$ for simplicity, we reparametrize the spatial coordinate as

$$z = \int_0^x \frac{du}{\sqrt{2D(u)}} \quad (4.78)$$

(i.e. we are interested in the process $Z(t) = \psi(X(t))$ where $\psi(x) = \int_0^x du / \sqrt{2D(u)}$).

b) Deduce the FPE for the distribution $Q_t(z)$ of $Z(t)$.

c) We first consider the case where the mapping $x \mapsto z$ with (4.78) maps $\mathbb{R}$ onto itself. Give an example of such $D(x)$. Give the propagator $Q_t(z|z_0)$ and deduce $P_t(x|x_0)$.

d) We now discuss the case where the mapping (4.78) maps $\mathbb{R}$ onto a finite interval $] -a, +a[$. For a diffusion of the form $D(x) = (1 + |x|)^\mu$, how should one choose μ ?

What is the domain of definition for $Q_t(z)$ in this case ? What is the expected distribution when $t \rightarrow \infty$? What is the related $P_t(x)$?

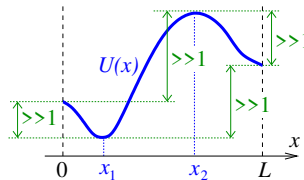
Compare to the discussion of Exercise ??.

✎ **Exercise 4.11 FPE on $\mathbb{R}$ for a non confining potential:** Consider the FPE $\partial_t P_t(x) = D \partial_x^2 P_t(x) + \partial_x[V'(x)P_t(x)]$ on $\mathbb{R}$ such that the drift $F(x) = -V'(x)$ drives the particle from $-\infty$ to $+\infty$. This requires that $V(x \rightarrow \pm\infty) \rightarrow \mp\infty$.

- 1/ Give an example of $V(x)$ and discuss the typical trajectories.
- 2/ Argue that $\mathcal{G}^T P = 0$ has two independent solutions.
- 3/ Show that the equilibrium solution is not normalisable and find the expression of the second solution (under the form of an integral).
- 4/ **Condition for the NESS**
 - a) If the stationary solution exists, using the expression found above, show that it presents the asymptotic behaviour $P_{\text{NESS}}(x) \simeq J/F(x)$ for $x \rightarrow +\infty$.
 - b) Deduce the condition for existence of the stationary state for the non confining potential.
 - c) Give an example of non confining drift with allows for a stationary state, and an example which does not.
- 5/ Compare with the results of Exercise 2.17 page 40.

✎ **Exercise 4.12 Steady state for periodic boundary conditions :** This exercise generalizes exercise 4.4. We consider the diffusion in a finite interval for periodic boundary conditions in a more general situation and discuss the nature of the steady state and the condition for equilibrium. We consider the general FPE $\partial_t P_t(x) = -\partial_x [F(x)P_t(x)] + \partial_x^2 [D(x)P_t(x)]$ for $x \in [0, L]$ with periodic boundary conditions.

- a) Write the differential equation for the stationary state $P_*(x)$. Give the general solution in terms of the “effective potential” $U(x) \stackrel{\text{def}}{=} -\int_0^x dy F(y)/D(y)$, which is assumed continuous in $]0, L[$ (i.e. $F(x)$ has no δ -function). If $U(x)$ is discontinuous, the only allowed discontinuity is at the boundary, i.e. $\Delta U = U(L) - U(0)$ may differ from zero.
- b) Impose the periodic boundary conditions on the steady state. Deduce its explicit expression, in terms of $U(x)$ and the steady current J .
- c) What is the condition for an equilibrium solution ?
- d) What condition provides the expression of the current (in terms of $F(x)$ and $D(x)$) ?
- e) **Application :** give the explicit form of $P_*(x)$ and J when $D(x) \rightarrow D$ and $F(x) \rightarrow \mu$ are constant. Deduce J .
- f) Using the expression of the current (question d/), find an approximation of J for the potential with the following form :



What controls the sign of the current ?

✎ **Exercise 4.13 First passage time for a constant drift :** We consider the trapping by a constant drift $F(x) = -\mu$. The particle starts from $x_0 \in [0, b[$ with a reflection boundary at $x = 0$. The boundary at b is absorbing.

- a) Compute the mean first passage time $T_1(x_0)$.
- b) Discuss the result : consider limiting cases (i) $\mu b/D \ll 1$, (ii) $\mu b/D \gg 1$ for $\mu > 0$, (iii) $|\mu|b/D \gg 1$ for $\mu < 0$.

✎ **Exercise 4.14 First passage time for $D \rightarrow D(x)$:** Generalize (4.71) for a x -dependent diffusion constant $D \rightarrow D(x)$:

- a) give the formula related to both the Itô and the Stratonovich SDE.
- b) Consider the FPE $\partial_t P_t(x) = \partial_x^2 [D(x)P_t(x)]$ (driftless case) for the reflection at $a = 0$ and

a diffusion constant $D(x) = \frac{1}{2}(1+x)^\mu$. Discuss $T_1(x_0)$ in the limit $b \rightarrow \infty$ (compare with the discussion of Exercise 4.10).

✎ **Exercise 4.15 NESS on $\mathbb{R}$ and the time needed to go from $-\infty$ to $+\infty$:** We consider a diffusion on $\mathbb{R}$ for generator $\mathcal{G} = D(x)\partial_x^2 - V'(x)\partial_x$, such that the NESS exists (see Exercise 4.11 when $D(x) \rightarrow D$). We study the case where the potential drives the process from $-\infty$ to $+\infty$: for example, for a uniform diffusion, when the drift is $F(x) = cx^2$, i.e. $V(x) = -\frac{1}{3}cx^3$.

a) Give an integral representation of the averaged time $T_1(x_0)$ needed to go from x_0 to $+\infty$.
Hint : you may consider a reflecting boundary at $a \rightarrow -\infty$ and an absorbing boundary at $b \rightarrow +\infty$.

b) Compare the averaged time and the current J related to the NESS (4.22).

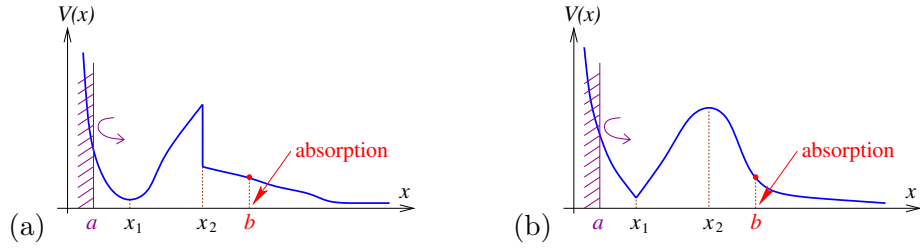


Figure 4.7: Two other types of trapping potentials.

✎ **Exercise 4.16 Lifetimes of metastable states:** We have obtained above the following formula for the average lifetime of a metastable state corresponding to the well of Fig. 4.5 : $\langle T_{x_0} \rangle \simeq \frac{2\pi}{\sqrt{-V''(x_1)V'''(x_2)}} \exp \left\{ \frac{V(x_2) - V(x_1)}{D} \right\}$, valid in the $D \rightarrow 0$ limit.

Derive some analogous formulae for the two potentials of Fig. 4.7.

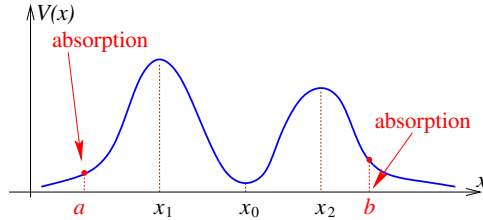


Figure 4.8: Two absorbing boundaries.

✎ **Exercise 4.17 First passage time in dimension d :** We consider the problem of first passage time in dimension $d > 1$: a diffusive particle submitted to a centro-symmetric drift $\vec{F}(\vec{r}) = -V'(r)\vec{u}_r$ where $\vec{u}_r$ is the radial unit vector. The forward generator of the diffusion in $\mathbb{R}^d$ is

$$\mathcal{G}^T = D\Delta - \vec{\nabla} \cdot \vec{F}. \quad (4.79)$$

The particle starts from $\vec{r}_0$ and we ask the question : when does it reach a sphere of radius $b < r_0 = \|\vec{r}_0\|$ for the first time ?

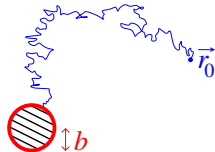


Figure 4.9: First passage on a sphere of radius b .

a) Show that the moments of the first passage time obey the differential equation

$$\left[D \left(\frac{d^2}{dr^2} + \frac{d-1}{r} \frac{d}{dr} \right) - V'(r) \frac{d}{dr} \right] T_n(r) = -n T_{n-1}(r) \quad (4.80)$$

Find an integral representation for $T_1(r_0)$.

b) When the dimension is increased, does the first passage time increases or decreases ?

c) Consider the potential $V(r) = \frac{k}{d} r^d$ in dimension d . Compute $T_1(r_0)$ and discuss the $b \rightarrow 0$ limit.

5 Linear response theory

Previously, we have been mostly interested to present some tools allowing to analyze the properties of stochastic processes, i.e. to follow a more *phenomenological* approach (with the exception of § page 10). In this last paragraph of this first part of the lectures, we are going to follow a more microscopic approach : we will however restrict ourselves to the study of **small disturbances on the top of equilibrium**, i.e. to the “linear regime”. Our purpose is to describe the situation represented schematically in Fig. 5.1.

Excitation $\longrightarrow$ **System** $\longrightarrow$ Measure of the response

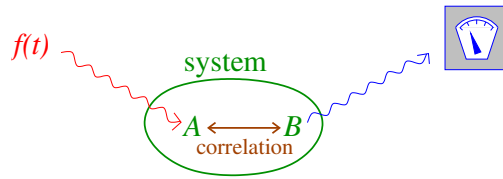


Figure 5.1: *Schematic representation of the situation under consideration : an excitation (external perturbation) acts on the system. A force $f(t)$ is coupled to an observable A of the system and another observable B is measured. The two observables are in general coupled by the time dynamics.*

A practical motivation could be to describe a bit more precisely the process of the measurement of an equilibrium property : the standard scheme to perform a measurement on a system at equilibrium consist in the introduction of a “small” perturbation (excitation) and the measurement of the response of the system (ex: an atomic vapor on which light is sent and which re-emit light by fluorescence).

First (§ 5.2), we start with a semi-phenomenological description based on thermodynamic properties (§ 5.1). In a second step (§ 5.3 to 5.5), we will develop the linear response theory.

5.1 Theory of thermodynamic fluctuations

This § was not discussed in the lectures due to lack of time.

Before entering into the (microscopic) approach of the linear response theory, it is useful to start with the more phenomenological approach of the thermodynamics of irreversible processes. We first start with the theory of thermodynamic fluctuations, which was developed by Einstein in 1910, among others [39]. In equilibrium thermodynamics, a fundamental function encoding all thermodynamic properties of a system is the entropy, which is an extensive function of a set of extensive variables (energy, number of particles, etc) characterizing the thermal state of the system :

$$S(\{X_i\}) \quad (5.1)$$

If the system is isolated, these extensive variables are fixed, however, if one considers extensive quantities characterizing a subpart of the system, there exist exchanges among different subparts : e.g. exchanges of energies, while the total energy of the isolated system is kept constant.

Conjugate thermodynamic forces : To each extensive variable X_i , we can associate an intensive conjugate force :

$$F_i = -\frac{\partial S}{\partial X_i} \quad (5.2)$$

Examples :

Observable X_i	force F_i
Energy E	$-1/T$
Volume V	$-p/T$
Number N_a	μ_a/T

In particular, for a simple fluid made of a mixture of s species we have

$$dS(E, V, \{N_a\}) = \frac{1}{T} dE + \frac{p}{T} dV - \sum_{a=1}^s \frac{\mu_a}{T} dN_a \quad (5.3)$$

Note that extensivity $S(\{\lambda X_i\}) = \lambda S(\{X_i\})$ implies

$$S(\{X_i\}) = - \sum_j X_j F_j(\{X_i\}) \quad (5.4)$$

a) Preliminary – the thermal contact :

As a preliminary, let us recall the analysis of the thermal contact between two subparts of an isolated system [50]. Denote by $S(E)$ the entropy of the part of interest and $S_{\text{ext}}(E_{\text{tot}} - E)$ the entropy of the remaining of the system. $S_{\text{tot}}(E) = S(E) + S_{\text{ext}}(E_{\text{tot}} - E)$ is the entropy of the isolated system for a fixed value E (here $S_{\text{tot}}(E)$ is the reduced entropy). The fundamental postulate of statistical physics provide the distribution of the energy E as

$$w(E) \propto e^{S_{\text{tot}}(E)} \quad (5.5)$$

(for clarity I set $k_B = 1$). We introduce the “affinity”

$$\phi(E) \stackrel{\text{def}}{=} -\frac{\partial S_{\text{tot}}(E)}{\partial E} = -\frac{1}{T(E)} + \frac{1}{T_{\text{ext}}(E_{\text{tot}} - E)} \quad (5.6)$$

which is the difference of the two ”forces”, involving here the microcanonical temperatures T and T_{ext} are characterizing the two sub-systems. The equation giving the maximum of the distribution correspond to the vanishing of the affinity

$$\phi(E) = 0 \quad \Rightarrow E = \bar{E} \quad (5.7)$$

and is also interpreted as the condition for thermal equilibrium $T = T_{\text{ext}}$.

Consider a thermal fluctuation

$$\delta E = E - \bar{E} \quad (5.8)$$

then we can linearize the affinity $\phi(\bar{E} + \delta E) \simeq \kappa \delta E$ hence the probability of a fluctuation is

$$w \propto e^{\delta S_{\text{tot}}} \quad \text{with } \delta S_{\text{tot}} \simeq -\frac{1}{2} \kappa \delta E^2 \quad (5.9)$$

Here the coefficient κ has a clear interpretation

$$\kappa = \phi'(\bar{E}) = \frac{1}{T(\bar{E})^2} \left(\frac{1}{C_V(\bar{E})} + \frac{1}{C_V^{\text{ext}}(E_{\text{tot}} - \bar{E})} \right) \simeq \frac{1}{T(\bar{E})^2 C_V(\bar{E})} \quad (5.10)$$

where the second term can be neglected if the subsystem is much smaller than the external part. With this assumption, we can write the probability in terms of a function characterizing the subsystem alone

$$w \propto e^{-\beta \mathcal{F}} \quad \text{with } \mathcal{F} = E - TS(E) \quad (5.11)$$

where T is here the temperature of the external and $\mathcal{F}$ the free energy of the subpart of interest.

Since there is a bijection between the energy and the temperature, $\delta E \simeq C_V \delta T$, we can as well express the fluctuation of energy in terms of the temperature

$$w \propto e^{\delta S_{\text{tot}}} \quad \text{with } \delta S_{\text{tot}} \simeq -\frac{1}{2\kappa} \delta T^2 = -\frac{C_V}{2T^2} \delta T^2 \quad (5.12)$$

thus the temperature fluctuations are

$$\langle \delta T^2 \rangle = \frac{k_B}{C_V} T^2 \quad (5.13)$$

where I have reintroduced the Boltzmann constant. I recall that C_V is here the heat capacity of the subpart in which the temperature fluctuations take place.

b) Affinities :

We now generalize these ideas to a set of extensive observables X_i . We consider a spontaneous thermal fluctuation

$$x_i = X_i - \bar{X}_i \quad (5.14)$$

and introduce the affinities corresponding to these observables

$$\phi_i \stackrel{\text{def}}{=} -\frac{\partial S_{\text{tot}}}{\partial X_i} = F_i - F_i^{\text{ext}} \quad (5.15)$$

Equilibrium state is characterised by the vanishing of all affinities $\phi_i = 0$.

In general we can write the entropy variation around its maximum (corresponding to the equilibrium state) as

$$\delta S_{\text{tot}} \simeq -\frac{1}{2} \sum_{i,j} \kappa_{ij} x_i x_j \quad (5.16)$$

where the coefficients κ_{ij} are encoded in the entropy function, the fundamental function characterizing the thermodynamic properties of the system, which is assumed known. Hence thermodynamic fluctuations are characterised by the Gaussian measure

$$w \propto e^{\delta S_{\text{tot}}} = e^{-\frac{1}{2} \sum_{i,j} \kappa_{ij} x_i x_j} \quad (5.17)$$

The affinities take the form

$$\phi_i = \sum_j \kappa_{ij} x_j \quad (5.18)$$

As a result of general properties of the Gaussian measure we have

$$\langle x_i x_j \rangle = (\kappa^{-1})_{ij} \quad (5.19)$$

(see appendix below). Using the linear relation between affinities and thermal fluctuations of observables, we get the correlator

$$\langle x_i \phi_j \rangle = \delta_{ij} \quad (5.20)$$

and

$$\langle \phi_i \phi_j \rangle = \kappa_{ij} . \quad (5.21)$$

Simple consequence : Let us apply Eq. (5.20) to the three extensive variables (E, V, N) , which are conjugated to (T, p, μ) , respectively. The relation shows that each extensive variable is only correlated with its conjugated force, and not forces conjugated to other extensive variables. For example V and T are uncorrelated, $\langle \delta T \delta V \rangle = 0$, etc.

It is also interesting to split the variation of entropy in two parts

$$\delta S_{\text{tot}} = \delta S + \delta S_{\text{exch}} = \delta S + \sum_i F_i^{\text{ext}} \delta X_i \quad (5.22)$$

where the second term is the entropy exchanged between the system and the external. Note that in [39], the variation of entropy δS_{tot} is denoted δS_{int} as it is the entropy variation relative to the changes internal to the system (energy fluctuation of the system, etc).

Application : For example, if we consider the entropy as a function of the energy and the volume, $S(E, V)$, this gives the form

$$w \propto \exp - \frac{\delta E - T \delta S + p \delta V}{T} = e^{-\beta \delta \mathcal{G}}, \quad (5.23)$$

where $\mathcal{G}$ is the free enthalpy. Expansion leads to

$$w \propto \exp \left\{ -\frac{C_V \delta T^2}{2T^2} - \frac{\delta V^2}{2TV \kappa_T} \right\} \quad (5.24)$$

where $\kappa_T \stackrel{\text{def}}{=} -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T$ is the isothermal compressibility, which controls the volume fluctuations $\langle \delta V^2 \rangle = TV \kappa_T$.

Appendix : Gaussian integrals in $\mathbb{R}^N$ and Wick theorem

Consider the integral

$$\mathcal{N}^{-1} = \int_{\mathbb{R}^N} d^N X e^{-\frac{1}{2} X^T A X} \quad (5.25)$$

where A is a real symmetric matrix. One can perform a rotation $X = \mathcal{O}Y$ which diagonalizes the matrix, $A = \mathcal{O}D\mathcal{O}^T$ with $D = \text{diag}(\lambda_1, \dots, \lambda_N)$. Jacobian of the transformation equals unity $J = |DX/DY| = |\det(\mathcal{O})| = 1$. This makes clear that the integral exists if the matrix is positive $A > 0$ (meaning $\lambda_i > 0 \forall i$). After diagonalization, the integral is separable, thus $\mathcal{N}^{-1} = \prod_i \sqrt{2\pi/\lambda_i} = (2\pi)^{N/2} / \sqrt{\det A}$.

Introduce the vector $B \in \mathbb{R}^N$ and the function

$$G(B) = \mathcal{N} \int_{\mathbb{R}^N} d^N X e^{-\frac{1}{2} X^T A X + B^T X} = \langle e^{B^T X} \rangle \quad (5.26)$$

which is interpreted as the generating function of the Gaussian variables X_i as derivations produce the correlation functions $\partial_{i_1} \dots \partial_{i_m} G(B)|_{B=0} = \langle X_{i_1} \dots X_{i_m} \rangle$. A simple manipulation is

$$X^T A X - 2B^T X = (X - A^{-1}B)^T A (X - A^{-1}B) - B^T A^{-1}B \quad (5.27)$$

leading to

$$G(B) = e^{\frac{1}{2} B^T A^{-1} B} \quad (5.28)$$

In particular we deduce the relation for the two point correlations $\langle X_i X_j \rangle = \frac{\partial^2 G(B)}{\partial B_i \partial B_j} \big|_{B=0}$:

$$\boxed{\langle X_i X_j \rangle = (A^{-1})_{ij}} \quad (5.29)$$

We conclude that the correlations of the Gaussian variable is already almost readable on the Gaussian measure itself $P(X) \propto \exp\{-\frac{1}{2}X^T A X\}$. This is a very general and important result.

We can deduce the **Wick theorem**

$$\langle X_1 \cdots X_{2n} \rangle = \sum_{\text{contractions}} \langle X_{i_1} X_{j_1} \rangle \cdots \langle X_{i_n} X_{j_n} \rangle \quad (5.30)$$

where the sum runs over the $(2n-1)!!$ pair contractions. Example : for $2n = 4$, one needs to consider the $(4-1)!! = 3$ contractions

$$\langle X_1 X_2 X_3 X_4 \rangle = \langle X_1 X_2 \rangle \langle X_3 X_4 \rangle + \langle X_1 X_3 \rangle \langle X_2 X_4 \rangle + \langle X_1 X_4 \rangle \langle X_2 X_3 \rangle \quad (5.31)$$

The Wick theorem has many occurrences and applications : in probability, in statistical physics, in statistical or quantum field theory.

5.2 Thermodynamics of irreversible processes

This § was not discussed in the lectures due to lack of time.

We now discuss the dynamics of observables when the system is driven slightly out-of-equilibrium (for example when inducing a current through a conductor by imposing a voltage drop). The main assumption is that the time scale which characterizes the dynamics is much longer than the time scale for relaxation towards equilibrium

$$\tau_{\text{dyn}} \gg \tau_{\text{relax}} \quad (5.32)$$

which ensures that the system follows equilibrium states described by equilibrium thermodynamic (in particular by the fundamental entropy function).

a) Fluxes

We introduce the flux related to the extensive variable X_i

$$J_i = \frac{dX_i}{dt} . \quad (5.33)$$

Denoting by $x_i(t) = X_i(t) - \overline{X_i}$ the deviation from equilibrium, we have also $J_i = \frac{dx_i}{dt}$. It is important to stress that although I use the same notation as the one used above for spontaneous thermal fluctuations, $x_i(t)$ designates here the change of the observable as a result of imposing a non zero affinity. The use of the same notation follows “**Onsager’s regression hypothesis**” (1930), *assuming that the relaxation of non equilibrium disturbance is governed by the same laws as the regression of spontaneous microscopic fluctuations* [7].

If the system remains close to the equilibrium, it is natural to *assume* that the fluxes are linear in the deviations to equilibrium, i.e.

$$\frac{dx_i}{dt} = - \sum_j \lambda_{ij} x_j \quad (\text{linear assumption}) . \quad (5.34)$$

It is important to keep in mind that at this level, contrary to coefficients κ_{ij} introduced above, which are encoded in the entropy function and can be deduced in terms of (equilibrium) thermodynamic properties, as it was illustrated above, the new phenomenological coefficients λ_{ij} characterize the dynamics and require further information. Using the linear relation with the affinities, it is conventional to write

$$J_i = \frac{dx_i}{dt} = \sum_j \gamma_{ij} \phi_j \quad (5.35)$$

where γ_{ij} are the so-called “*kinetic coefficients*”. The main object of the theory of irreversible processes is to find the relation between affinities and fluxes (in electronic devices, this corresponds to finding the relation between the voltage drop imposed by the external on the device and the induced current, i.e. a formula for the conductance in terms of the microscopic parameter and the geometry of the conductor). At this stage, the description remains phenomenological. The sets of coefficients are clearly related by

$$\gamma_{ij} = - \sum_k \lambda_{ik} (\kappa^{-1})_{kj} \quad (5.36)$$



Figure 5.2: *Lars Onsager (1903-1976), Nobel prize in chemistry 1968.*

Example : the discussion is a bit formal. Let us give a concrete example : consider a conductor with charge Q (the “observable” X). The electrostatic energy is $H = QV$ so that the potential V is the “conjugated force ϕ ”). The “flux J ” is the electric current $I = \frac{dQ}{dt}$ and thus the kinetic coefficient is simply the conductance (inverse of resistance)

$$\gamma \longrightarrow G \quad (5.37)$$

as we usually writes $I = GV$).

b) Onsager symmetry relation

We now state the Onsager principle (1931) of the symmetry of kinetic coefficients

$$\boxed{\gamma_{ij} = \gamma_{ji}} \quad (5.38)$$

which relies on the time reversal symmetry, at equilibrium, as we now show.

Proof : We introduce the correlation function

$$C_{ij}(t) = \langle x_i(t)x_j(0) \rangle \quad (5.39)$$

Assuming *time reversal symmetry* we have

$$\langle x_i(t)x_j(0) \rangle = \langle x_i(0)x_j(-t) \rangle \stackrel{\text{TRS}}{=} \langle x_i(0)x_j(t) \rangle \quad \Rightarrow \quad C_{ij}(t) = C_{ji}(t) . \quad (5.40)$$

Now we differentiate the relation

$$\left\langle \frac{dx_i(t)}{dt} x_j(0) \right\rangle = \left\langle \frac{dx_j(t)}{dt} x_i(0) \right\rangle \quad (5.41)$$

and we use Onsager's regression hypothesis, which allows to make use of the kinetic coefficients

$$\sum_k \gamma_{ik} \langle \phi_k(t)x_j(0) \rangle = \sum_k \gamma_{jk} \langle \phi_k(t)x_i(0) \rangle \quad (5.42)$$

Because the relation holds $\forall t$ we can write

$$\sum_k \gamma_{ik} \underbrace{\langle \phi_k(0)x_j(0) \rangle}_{=\delta_{jk}} = \sum_k \gamma_{jk} \underbrace{\langle \phi_k(0)x_i(0) \rangle}_{=\delta_{ik}} \quad (5.43)$$

leading to (5.38).

Remarks :

- A standard illustration is the symmetry between transport of particles and transport of energy. Transport of particles can be induced by a modulation of the electrochemical potential $\bar{\mu} = \mu + V(\vec{r})$, where $V(\vec{r})$ is the potential (in the presence of an external potential, the "force" conjugated to the local density is $\bar{\mu}$). Transport of energy can be induced by an imbalance of temperature (Fick's law). The local version gives the current of particles and the current of energy

$$\vec{J}_N = \gamma_{NN} \vec{\nabla} \left(\frac{\bar{\mu}}{T} \right) + \gamma_{NE} \vec{\nabla} \left(-\frac{1}{T} \right) \quad (5.44)$$

$$\vec{J}_E = \gamma_{EN} \vec{\nabla} \left(\frac{\bar{\mu}}{T} \right) + \gamma_{EE} \vec{\nabla} \left(-\frac{1}{T} \right) \quad (5.45)$$

The coefficient γ_{NN} is proportional to the diffusion constant (or the conductivity for charged particles) and the coefficient γ_{EE} to the thermal conductivity. The Onsager symmetry relation is $\gamma_{NE} = \gamma_{EN}$. Its existence is related to the duality of two effects : the Seebeck and the Peltier effects [39, 23].

- The Onsager symmetry relations (5.38) was given here for observables invariant under time reversal symmetry. In general the observables can have a specific symmetry under TRS :

$$x_i(-t) = \epsilon_i x_i(t) \quad \text{with } \epsilon_i = \pm 1 . \quad (5.46)$$

In the more general case, the Onsager symmetry relations take the form

$$\gamma_{ij}(\vec{B}, \vec{\Omega}) = \epsilon_i \epsilon_j \gamma_{ji}(-\vec{B}, -\vec{\Omega}) \quad (5.47)$$

where $\vec{B}$ is the magnetic field and $\vec{\Omega}$ the angular velocity of rotation.

- **Equilibrium *versus* out-of-equilibrium.**— We will make clear below that, although they characterize how the system responds when put slightly out-of-equilibrium, the kinetic coefficients are properties of the *equilibrium* state. Thermal equilibrium is a crucial assumption for the Onsager symmetry relations to hold. In the out-of-equilibrium situation, Onsager symmetry can be broken.
- **Linear response *versus* non linear response.**— Another formulation of the previous remark : the fluxes are non zero because finite affinities are imposed from the external, hence the fluxes are functions of the affinities : $J_i(\{\phi_j\})$. We have written above the fluxes as $J_i(\{\phi_j\}) = \sum_j \gamma_{ij} \phi_j$. Assuming that the response is linear is equivalent to say that the kinetic coefficients are properties of the system for $\phi_i = 0 \forall i$, $\gamma_{ij} = \mathcal{O}(\phi_k^0)$, i.e. that they are properties of the system *at equilibrium* (this is the essence of Onsager's regression hypothesis). Onsager symmetry relation holds for the linear response, however it has no reason to hold for the non-linear response, i.e. far from equilibrium.

An example was discussed in [42, 45] (and further in [49]) : whereas it is well known that the linear conductance of a conductor with two contacts is a symmetric function of the magnetic field, the interaction between electrons was shown to induce an asymmetry of the nonlinear response under magnetic field reversal. This was observed experimentally in [55, 3].

c) Entropy production

The entropy production corresponds to dissipation (cf. end of appendix p. 10)

$$\frac{dS_{\text{tot}}}{dt} = \sum_i \frac{\partial S_{\text{tot}}}{\partial X_i} \frac{dX_i}{dt} = \sum_i \phi_i J_i \quad (5.48)$$

Hence the entropy production is a quadratic form

$$\frac{dS_{\text{tot}}}{dt} = \sum_{ij} \gamma_{ij} \phi_i \phi_j \quad (5.49)$$

As a consequence of the 2nd "principle" of thermodynamic (demonstrated within the frame of statistical physics), $dS_{\text{tot}}/dt \geq 0$, we have

$$\gamma_{ii} \geq 0 \quad (5.50)$$

and $\gamma_{ii}\gamma_{jj} \geq \frac{1}{4}(\gamma_{ij} + \gamma_{ji})^2$. More generally γ_{ij} is a positive matrix.

Bibliography:

- The chapter 12 of the Landau & Lifshitz [19] (the unpleasant notation R_{min} is used for the free energy or the free enthalpy).
- The chapter 2 of the book by Pottier [39] is well written (although the notations can be a bit confusing). The local formulation is developed. The chapter 2 of Livi and Politi's book [23] discusses this matter but is less detailed.
- The chapter 6 of Le Bellac et al's book [21].

5.3 Correlation functions and response functions

Let us now enter into the heart of linear response theory. Being a microscopic approach, it should be based on a description as microscopic as possible : we adopt the frame of classical mechanics and consider the distribution function in phase space.

- Phase space : we denote by $\vec{\Gamma}$ a point (the “microstate”) in the D -dimensional phase space. For example, for a gas of N atoms, it is the vector $\vec{\Gamma} \equiv (\vec{r}_1, \dots, \vec{r}_N, \vec{p}_1, \dots, \vec{p}_N)$ with $D = 6N$ components.
- The dynamics of the system is controlled by the Hamiltonian $H(\vec{\Gamma})$.
- We adopt a probabilistic description and consider the distribution in phase space, denoted $\rho_t(\vec{\Gamma})$, which is the probability density in phase space at time t . It follows from the Hamiltonian equations of motion that it obeys the Liouville equation (see for example appendix of chapter 3 of [50])

$$\frac{\partial}{\partial t} \rho_t = \{H, \rho_t\} \quad (5.51)$$

where

$$\{A, B\} \stackrel{\text{def}}{=} \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right) \quad (5.52)$$

is a Poisson bracket.

- Finally, considering an observable $A(\vec{\Gamma})$ (for example the kinetic energy $H_{\text{kin}} = \frac{1}{2m} \sum_i \vec{p}_i^2$), the average at time t is given by

$$\langle A \rangle_t = \int d^D \vec{\Gamma} \rho_t(\vec{\Gamma}) A(\vec{\Gamma}) . \quad (5.53)$$

Here, the evolution is carried by the density. Below, it will be conceptually more simple to write the average differently, with the evolution carried by the observable :

$$\langle A \rangle_t = \int d^D \vec{\Gamma}_0 \rho_0(\vec{\Gamma}_0) A(\vec{\Gamma}(t)) \quad (5.54)$$

where $\vec{\Gamma}(t)$ is the trajectory such that $\vec{\Gamma}(0) = \vec{\Gamma}_0$. The distinction between (5.53) and (5.54) is similar to the difference between Schrödinger and Heisenberg pictures in quantum mechanics. Below I will rather use the notation $\langle A \rangle_t \equiv \langle A(t) \rangle$ (a more consistent notation should be $\langle A(\vec{\Gamma}(t)) \rangle$ but it is too heavy).

a) Equilibrium and static response

Consider a modification of the Hamiltonian

$$H_0(\vec{\Gamma}) \longrightarrow H_f(\vec{\Gamma}) = H_0(\vec{\Gamma}) - f A(\vec{\Gamma}) \quad (5.55)$$

where A is a certain “observable” and f the conjugate force (here in the sense of classical mechanics). I.e. the observable can be obtained by differentiation with respect to this parameter $A(\vec{\Gamma}) = -\frac{\partial}{\partial f} H_0(\vec{\Gamma})$. Assume canonical equilibrium

$$\rho^f(\vec{\Gamma}) = \frac{1}{Z_f} e^{-\beta H_f(\vec{\Gamma})} \quad \text{with } Z_f = \int d^D \vec{\Gamma} e^{-\beta H_f(\vec{\Gamma})} . \quad (5.56)$$

Consider the average of another observable

$$\langle B \rangle_f = \int d^D \vec{\Gamma} \rho^f(\vec{\Gamma}) B(\vec{\Gamma}) \quad (5.57)$$

Question : given $\langle B \rangle_0 = \int d^D \vec{\Gamma} \rho^0(\vec{\Gamma}) B(\vec{\Gamma})$, can we study the variation of the average due to the introduction of the force f ? A motivation can be that we are able to compute $\langle B \rangle_0$, but not $\langle B \rangle_f$. As a preliminary, let us expand the partition Z_f in powers of f :

$$Z_f \simeq \int d^D \vec{\Gamma} e^{-\beta H_0(\vec{\Gamma})} \left(1 + \beta f A(\vec{\Gamma}) + \dots \right) = Z_0 (1 + \beta f \langle A \rangle_0 + \dots) . \quad (5.58)$$

Similarly, we can expand the average

$$\langle B \rangle_f \simeq \int d^D \vec{\Gamma} B(\vec{\Gamma}) \frac{e^{-\beta H_0}}{Z_0} \frac{1 + \beta f A(\vec{\Gamma}) + \dots}{1 + \beta f \langle A \rangle_0 + \dots} \quad (5.59)$$

Finally we can write

$$\langle B \rangle_f = \langle B \rangle_0 + f \chi_{BA}^{\text{stat}} + \mathcal{O}(f^2) \quad (5.60)$$

where

$$\chi_{BA}^{\text{stat}} = \beta (\langle BA \rangle_0 - \langle B \rangle_0 \langle A \rangle_0) \quad (5.61)$$

is the “static response function”. At lowest order in f , the properties of observables in the presence of the force are controlled by a *correlator* characterizing the equilibrium state ρ^0 .

Example: consider a magnetic system with magnetic energy $H_{\text{magn}} = -\mathcal{B} M$ where M is the magnetization. The **magnetic susceptibility** is the response of the magnetization to the magnetic field $\langle M \rangle_{\mathcal{B}} \simeq \chi \mathcal{B}$ for $\mathcal{B} \rightarrow 0$. Application of the formula shows that the susceptibility is related to the fluctuations of magnetization :

$$\chi = \frac{\langle \delta M^2 \rangle_0}{k_B T} \quad (5.62)$$

(cf. chap. 10 of [50]).

A Mathematical tools

A.1 Linear differential equations with source terms

First order.— First consider the simple differential equation

$$y'(x) - \lambda y(x) = s(x) \quad (\text{A.1})$$

where λ and $s(x)$ are given. The solution of the homogeneous equation is $y(x) = A e^{\lambda x}$. Use the "variation of the constant's method" : search a particular solution under the form $y(x) = A(x) e^{\lambda x}$, which leads to $A'(x) = s(x) e^{-\lambda x}$, i.e. $A(x) = \int_0^x dt s(t) e^{-\lambda t}$. Hence the general solution is

$$y(x) = y(0) e^{\lambda x} + \int_0^x dt s(t) e^{\lambda(x-t)} \quad (\text{A.2})$$

You can check that the method can be extended to the case where $\lambda \rightarrow \lambda(x)$ in the differential equation (A.1). Then

$$y(x) = y(0) e^{\int_0^x du \lambda(u)} + \int_0^x dt s(t) e^{\int_t^x du \lambda(u)} \quad (\text{A.3})$$

a) Fourier transform on $\mathbb{R}$

Consider a complex function f defined on $\mathbb{R}$. Its Fourier transform is defined as

$$\hat{f}(k) = \int_{\mathbb{R}} dx f(x) e^{-ikx} \quad \text{and} \quad f(x) = \int_{\mathbb{R}} \frac{dk}{2\pi} \hat{f}(k) e^{ikx} \quad (\text{A.4})$$

the inverse Fourier transform is recovered by using

$$\int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx} = \delta(x) \quad (\text{A.5})$$

You should now the basic properties of Fourier transform

$$\mathcal{F}_k[f'(x)] = ik \hat{f}(k), \quad (\text{A.6})$$

$$\hat{f}(ak) = \mathcal{F}_k[(1/a) f(x/a)], \quad (\text{A.7})$$

$$\mathcal{F}_k[f * g] = \hat{f}(k) \hat{g}(k), \quad \text{etc.} \quad (\text{A.8})$$

We can recover the standard properties of the Fourier transform. For instance, the Parseval-Plancherel relation

$$\int_{\mathbb{R}} dx |f(x)|^2 = \int_{\mathbb{R}} \frac{dk}{2\pi} |\hat{f}(k)|^2 \quad (\text{A.9})$$

etc.

b) Discrete Fourier transform (over a finite interval)

Consider a function $f(x)$ defined on a finite interval $x \in [0, L]$ (the function can be a periodic function with period L). For a bounded domain, the wave vectors are quantized, hence the function can be decomposed over a countable basis of plane waves

$$u^{(n)}(x) = e^{ik_n x} \quad \text{for } k_n = \frac{2n\pi}{L} \text{ with } n \in \mathbb{Z}. \quad (\text{A.10})$$

We easily check the orthonormalisation condition

$$\int_0^L \frac{dx}{L} u^{(n)}(x)^* u^{(m)}(x) = \int_0^L \frac{dx}{L} e^{i(k_m - k_n)x} = \delta_{n,m} \quad (\text{A.11})$$

Thus Fourier transform takes the form

$$f(x) = \frac{1}{L} \sum_{n \in \mathbb{Z}} \hat{f}_n e^{ik_n x} \quad \text{where} \quad \hat{f}_n = \int_0^L dx f(x) e^{-ik_n x} = \langle u^{(n)} | f \rangle \quad (\text{A.12})$$

If we take the limit $L \rightarrow \infty$, the spectrum of wave vectors becomes dense and we recover the continuous Fourier transform, using $\frac{1}{L} \sum_{k_n} \rightarrow \int_{\mathbb{R}} \frac{dk}{2\pi}$.

Note that

$$\int_0^L dx |f(x)|^2 = \frac{1}{L} \sum_{n \in \mathbb{Z}} |\hat{f}_n|^2. \quad (\text{A.13})$$

c) Fourier transform of a discrete function

If we consider a function f_x defined over $\mathbb{Z}$ (on a lattice), the basis of harmonic functions are plane waves $u_x^{(k)} = e^{ikx}$ where the wave vector varies continuously over a bounded domain, the "Brillouin zone" $k \in]-\pi, +\pi]$ (because $u_x^{(k+2\pi)} = u_x^{(k)}$ for $x \in \mathbb{Z}$). As a result

$$f_x = \int_{-\pi}^{+\pi} \frac{dk}{2\pi} \hat{f}(k) e^{ikx} \quad \text{where} \quad \hat{f}(k) = \sum_{x \in \mathbb{Z}} f_x e^{-ikx} \quad (\text{A.14})$$

The passage between the two is now ensured by the Poisson formula

$$\sum_{n \in \mathbb{Z}} \delta(k - 2\pi n) = \frac{1}{2\pi} \sum_{x \in \mathbb{Z}} e^{ikx} \quad (\text{A.15})$$

(because k is in the Brillouin zone, we only need the $n = 0$ term).

It is also possible to recover the Fourier transform for continuous functions by introducing a lattice spacing a (writing now that $x/a \in \mathbb{Z}$). The Brillouin zone is then $k \in]-\pi/a, \pi/a]$. In the limit $a \rightarrow 0$ we recover the Fourier transform.

d) Fourier transform of a discrete function defined over a finite set

If we now define a discrete function f_x over a finite set $x \in \{1, 2, \dots, L\}$, the wave vector is both quantized (finite volume) and bounded (lattice problem) :

$$k_n = 2\pi n/L \quad \text{with} \quad n = -L/2 + 1, \dots, -1, 0, 1, \dots, L/2 \in]-\pi, +\pi]$$

(for L even).

Preliminary.— consider the N roots of the identity, solutions of $z^N = 1$,

$$z_k = e^{2i\pi k/N} \quad \text{for } k = 0, 1, \dots, N-1 \quad (\text{A.16})$$

Using that the characteristic polynomial is

$$P(z) = z^N - 1 = \prod_{k=0}^{N-1} (z - z_k) \quad (\text{A.17})$$

$\prod_k (z - z_k)$ is a polynomial of degree N with only two terms. The z^1 coefficient being zero, we have $\sum_k z_k = 0$. Similarly we can prove $\sum_k z_k^n = N \delta_{n,0}$ for $n \in \{0, 1, \dots, N-1\}$, i.e. more explicitly

$$\frac{1}{N} \sum_{k=0}^{N-1} e^{2i\pi nk/N} = \delta_{n,0}. \quad (\text{A.18})$$

This relation can be used for the Fourier transform.

Fourier transform.— We have now

$$f_x = \frac{1}{L} \sum_{n=1}^L \hat{f}_n e^{2i\pi nx/L} \quad \text{where} \quad \hat{f}_n = \sum_{x=1}^L f_x e^{-2i\pi nx/L} \quad (\text{A.19})$$

A.2 Poisson formulae

Consider a function f defined on $\mathbb{R}$ and its Fourier transform $\hat{f}$, then

$$\boxed{\sum_{n \in \mathbb{Z}} f(n) = \sum_{n \in \mathbb{Z}} \hat{f}(2\pi n)} \quad \text{where} \quad \hat{f}(k) = \int_{\mathbb{R}} dx f(x) e^{-ikx}. \quad (\text{A.20})$$

In particular

$$\sum_{n \in \mathbb{Z}} \delta(x - n) = \sum_{n \in \mathbb{Z}} e^{2i\pi nx} \quad (\text{A.21})$$

✎ **Exercise A.1 :** Check that

$$\Theta(y|\alpha, \eta) \stackrel{\text{def}}{=} \sum_{n \in \mathbb{Z}} e^{2i\pi n \eta} e^{-\pi^2 (n+\alpha)^2 y} = \frac{1}{\sqrt{\pi y}} \sum_{n \in \mathbb{Z}} e^{2i\pi (n-\eta)\alpha} e^{-\frac{(n-\eta)^2}{y}}, \quad (\text{A.22})$$

This sum is related to the Jacobi theta function (DLMF, § 20) $\theta_3(z, q) = \sum_n q^{n^2} e^{2inz}$, i.e. $\Theta(y|0, \eta) = \theta_3(\pi\eta, e^{-\pi^2 y})$.

A.3 Asymptotics of integrals

One frequently deals with integrals involving large parameters (furthermore, many useful special functions are defined through nice integral representations). Here I recall two methods allowing to extract some asymptotic behaviour.

a) The Laplace method

Consider a monotonously increasing function $\varphi(x)$ and the integral $\int_0^\infty dx e^{-\lambda\varphi(x)}$. When $\lambda \rightarrow +\infty$, one expects the exponential to decay fast, on scale $\sim 1/(\lambda\varphi'(0)) \rightarrow 0$, and the integral is dominated by the boundary. Note that in the expansion $e^{-\lambda\varphi(x)} = e^{-\lambda\varphi(0)} \exp\{-\lambda\varphi'(0)t - \lambda\varphi''(0)t^2/2 + \dots\}$, the exponential $e^{-\lambda\varphi''(0)t^2/2}$ decays over a *larger* scale, $\sim 1/(\lambda\varphi''(0))^{1/2}$. In conclusion, adding a smooth function $g(x)$ in the integral, we can write

$$I(\lambda) = \int_0^\infty dx g(x) e^{-\lambda\varphi(x)} \underset{\lambda \rightarrow +\infty}{\simeq} \frac{g(0)}{\lambda\varphi'(0)} e^{-\lambda\varphi(0)} \quad (\text{A.23})$$

Note that if $g(x)$ vanishes, we can extend the method. For example, a similar expansion gives

$$I(\lambda) = \int_0^\infty dx g(x) e^{-\lambda\varphi(x)} \underset{\lambda \rightarrow +\infty}{\simeq} \frac{g'(0)}{[\lambda\varphi'(0)]^2} e^{-\lambda\varphi(0)} \quad \text{for } g(x) \simeq g'(0)x \text{ for } x \rightarrow 0. \quad (\text{A.24})$$

Remark : a systematic expansion under these lines usually produce an asymptotic series. For example, one can apply the method to get the asymptotic of the exponential integral :

$$E_1(z) \stackrel{\text{def}}{=} \int_z^\infty \frac{dt}{t} e^{-t} \quad (\text{A.25})$$

One obtains $E_1(z) \simeq (1/z)e^{-z}$ for $z \rightarrow +\infty$. This is the first term of the asymptotic series (series with zero convergence radius)

$$E_1(z) \underset{z \rightarrow \infty}{=} \frac{e^{-z}}{z} \left(\sum_{k=0}^n (-1)^k \frac{k!}{z^k} + \mathcal{O}(|z|^{-n-1}) \right) \quad (\text{A.26})$$

(valid for $|\arg(z)| \leq \pi - \delta$ with $\delta > 0$). ⁵²

b) The steepest descent method (saddle point approximation)

Another frequently encountered case is an integral of the form $\int_a^b dx e^{-\lambda \varphi(x)}$ where $\lambda \in \mathbb{R}$ is a large parameter and $\varphi(x)$ a real function with one absolute minimum at $x_* \in]a, b[$ sufficiently far from the boundaries, with $\varphi''(x_*) > 0$. In the $\lambda \rightarrow +\infty$ limit, the exponential is sharply peaked around x_* and we can expand the function around it, which leads to a Gaussian integral. As a result

$$I(\lambda) = \int_a^b dx e^{-\lambda \varphi(x)} \underset{\lambda \rightarrow +\infty}{\simeq} \sqrt{\frac{2\pi}{\lambda \varphi''(x_*)}} e^{-\lambda \varphi(x_*)}. \quad (\text{A.27})$$

Remarks :

- When $\varphi(x)$ is analytic, contour deformations are allowed, which allows to pass through a saddle point not on the original contour (the real axis) but somewhere else in the complex plane.
- The method also applies to integral of the type $I(\lambda) = \int_a^b dx e^{-i\lambda \varphi(x)}$ where λ and $\varphi(x)$ are real. In this case one should take into account the contributions of all stationary points along the contour, i.e. both maxima and minima of $\varphi(x)$. Then, the method is called the “*stationary phase method*”.

✎ **Exercise A.2 :** Extend the method when $\varphi''(x_*) = 0$, $\varphi'''(x_*) = 0$ and $\varphi^{(4)}(x_*) > 0$.

✎ **Exercise A.3 Asymptotic of the MacDonald function :** The modified Bessel equation is $z^2 y''(z) + z y'(z) - (\nu^2 + z^2) y(z) = 0$. A possible set of independent solutions are the modified Bessel function $I_\mu(z) = \sum_{n=0}^\infty \frac{(z/2)^{2n+\mu}}{n! \Gamma(\mu+n+1)}$ and the MacDonald function (Bessel function of third kind) $K_\mu(z) = \frac{\pi}{2 \sin \pi \mu} [I_{-\mu}(z) - I_\mu(z)]$ (the expression is valid for $\mu \notin \mathbb{Z}$). The first is regular for $z \rightarrow 0$ and grows exponentially at infinity $I_\mu(z) \sim e^{+z}$. The second is divergent for $z \rightarrow 0$ and decays exponentially at infinity. Given the integral representation

$$K_\nu(z) = \frac{1}{2} \left(\frac{z}{2} \right)^\nu \int_0^\infty \frac{dt}{t^{\nu+1}} e^{-t-z^2/4t} \quad \text{for } \text{Re } z > 0 \quad (\text{A.28})$$

Using the integral representation (A.28) of the MacDonald function, use the steepest descent method to get the asymptotic $K_\nu(z) \underset{z \rightarrow +\infty}{\simeq} \sqrt{\frac{\pi}{2z}} e^{-z}$.

⁵²You can get the series easily by introducing $E_k(z) \stackrel{\text{def}}{=} \int_z^{+\infty} \frac{dt}{t^k} e^{-t}$ and use the recurrence $E_n(z) = \frac{e^{-z}}{z^n} - \frac{n}{z} E_{n+1}(z)$

✎ **Exercise A.4** : Requirement of a contour deformation in the application of the steepest descent method appears when studying the Airy function

$$\text{Ai}(z) = \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{i(\frac{t^3}{3} + zt)} \quad (\text{A.29})$$

solution of the Airy equation $y''(z) = zy(z)$. We study the asymptotic for $z \rightarrow \pm\infty$. Find the saddle point(s) and deduce the asymptotics

$$\text{Ai}(z) \simeq \begin{cases} \frac{1}{2\sqrt{\pi} z^{1/4}} e^{-\frac{2}{3}z^{3/2}} & \text{for } z \rightarrow +\infty \\ \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos\left(\frac{2}{3}(-z)^{3/2} - \frac{\pi}{4}\right) & \text{for } z \rightarrow -\infty \end{cases} \quad (\text{A.30})$$

argue that only one saddle point controls the asymptotic for $z > 0$.

Hint : plot $\varphi(t)$ along the imaginary axis of the complex variable t .

A.4 Special functions

Special functions are very useful. You can find information in standard books [15, 2] or on the internet [1].

Euler Gamma function

any integral of the form $\int_0^\infty dx x^\alpha e^{-cx^\beta}$ can be related to the Euler Gamma function

$$\Gamma(z) = \int_0^\infty dt t^{z-1} e^{-t} \quad \text{for } \text{Re}(z) > 0. \quad (\text{A.31})$$

It can also be defined for $\text{Re}(z) \leq 0$, however it presents simple poles for $-n \in \mathbb{N}$.

Important property : $\Gamma(z+1) = z\Gamma(z)$.

Special values : $\Gamma(1) = 1$ and $\Gamma(1/2) = \sqrt{\pi}$.

From these, we immediatly deduce $\Gamma(n+1) = n!$ and $\Gamma(n + \frac{1}{2}) = 2^{-n}\sqrt{\pi}(2n-1)!!$.

Asymptotic is given by the Stirling formula for $z \gg 1$

$$\Gamma(z+1) \simeq \sqrt{2\pi z} z^z e^{-z}. \quad (\text{A.32})$$

✎ **Exercise A.5** : Demonstrate this result starting from the integral representation and using the steepest descent method (cf. Appendix b) page 159).

✎ **Exercise A.6** : Express the integral

$$\int_0^\infty dx x^\mu e^{-\frac{1}{2}ax^2} \quad (\text{A.33})$$

in terms of the Gamma function.

Digamma function : The Digamma function is $\psi(z) \stackrel{\text{def}}{=} \frac{d}{dz} \ln \Gamma(z) = \frac{\Gamma'(z)}{\Gamma(z)}$. As a result it obeys $\psi(z+1) = \psi(z) + \frac{1}{z}$.

One specific value is $\psi(1) = \mathbf{C} \simeq -0.577216$; this constant is known as the Euler-Mascheroni constant.

Euler Beta function

The Beta function is defined as

$$B(\mu, \nu) = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu + \nu)} . \quad (\text{A.34})$$

Useful integrals :

$$B(\mu, \nu) = \int_0^1 dt t^{\mu-1} (1-t)^{\nu-1} = 2 \int_0^{\pi/2} d\theta \sin^{2\mu-1} \theta \cos^{2\nu-1} \theta . \quad (\text{A.35})$$

Error function

The error function is the integral of the Gaussian function :

$$\text{erf}(z) \stackrel{\text{def}}{=} \frac{2}{\sqrt{\pi}} \int_0^z dt e^{-t^2} \quad (\text{A.36})$$

We also introduce the complementary error functions $\text{erfc}(z) = 1 - \text{erf}(z)$. Asymptotics :

$$\text{erfc}(z) \underset{z \rightarrow \infty}{\simeq} \frac{e^{-z^2}}{\sqrt{\pi}} \sum_{n=0}^N (-1)^n \frac{(1/2)_n}{z^{2n+1}} + R_N(z) \quad (\text{A.37})$$

where $(a)_n$ is the Pochhammer symbol.

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