Chapter 3

Diffusive Markov processes

3.1 Fokker-Planck equation

We will now present particular cases of the Chapman-Kolomogorov equation for homogeneous Markov processes that turn out to be very useful to describe many physical systems. From now on, we will only consider continuous Markov processes. They are said to be *diffusive* in the sense that the theory provides a generalization of Brownian diffusion to a large range of systems. The discrete-valued processes will be dealt with in the next chapter.

Let us come back to the Brownian motion and calculate the moments of the particle motion starting from an initial position x_0 at time $t_0 = 0$. According to equation (1.24), these moments read[1]

$$\begin{aligned}
\left\langle (\Delta x)^k \right\rangle_{x_0} &\equiv \int_{\mathbb{R}} \mathrm{d}x\, (x-x_0)^k P(x_0|x,t) \\
&= \int_{\mathbb{R}} \mathrm{d}x\, (x-x_0)^k \frac{1}{\sqrt{4\pi D t}} \mathrm{e}^{-\frac{(x-x_0)^2}{4Dt}} \\
&\overset{u=\frac{x-x_0}{\sqrt{2Dt}}}{=} (2Dt)^{k/2} \int_{\mathbb{R}} \mathrm{d}u\; u^k \frac{\mathrm{e}^{-u^2/2}}{\sqrt{2\pi}} \\
&= C(k) \times \begin{cases} 0, & k=1, \\ 2Dt, & k=2, \\ (2\pi t)^{k/2}, & k \geq 3, \end{cases}
\end{aligned} \tag{3.1}$$

where $C(k)$ can be calculated using the formula

$$\int_{\mathbb{R}} \mathrm{d}x\; x^n \mathrm{e}^{-ax^2} = \begin{cases} \frac{1}{a^{\frac{n+1}{2}}} \frac{(n-1)!!}{2^{\frac{n}{2}}} \sqrt{\pi}, & n \text{ even}, \\ 0, & n \text{ odd}. \end{cases} \tag{3.2}$$

The diffusive nature results in the fact that $\left\langle (\Delta x)^2 \right\rangle_{x_0}$ is of order t and that the higher-order moments $\left\langle (\Delta x)^k \right\rangle_{x_0}$, $k > 2$, tend to zero faster than t as $t \to 0$. These considerations lead to the following definition.

[1] If $t_0 \neq 0$, we just have to replace t by $t - t_0$ everywhere.

Definition 3.1 (Diffusive process) *A homogeneous Markov process is said to be diffusive if there exists two functions $a(x)$ and $b(x)$ such that the transition probability $P(x_0|x,t)$ satisfies*

$$\begin{aligned}
&(i)\ \ \langle \Delta x\rangle_{x_0} &&= \textstyle\int_{\mathbb{R}} \mathrm{d}x\,(x-x_0)P(x_0|x,t) &&\overset{t\sim 0}{=}\ a(x_0)t\ +\ \mathcal{O}\left(t^{\alpha}\right), &&\alpha>1,\\
&(ii)\ \ \langle (\Delta x)^2\rangle_{x_0} &&= \textstyle\int_{\mathbb{R}} \mathrm{d}x\,(x-x_0)^2P(x_0|x,t) &&\overset{t\sim 0}{=}\ b(x_0)t\ +\ \mathcal{O}\left(t^{\alpha}\right), &&\alpha>1,\\
&(iii)\ \left\langle (\Delta x)^k\right\rangle_{x_0} &&= \textstyle\int_{\mathbb{R}} \mathrm{d}x\,(x-x_0)^kP(x_0|x,t) &&\overset{t\sim 0}{=}\ \mathcal{O}\left(t^{\alpha}\right), &&\alpha>1,\ k>2.
\end{aligned}$$

The functions $a(x)$ and $b(x)$ are respectively called *drag* et *diffusion* functions of the process.

The transition probability $P(x_0|x,t)$ fulfills a second order differential equation called *Fokker-Planck equation*

$$\boxed{\frac{\partial}{\partial t}P(x_0|x,t) = -\frac{\partial}{\partial x}\big(a(x)P(x_0|x,t)\big) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\big(b(x)P(x_0|x,t)\big),} \tag{3.3}$$

with initial condition $P(x_0|x,t=0)=\delta(x-x_0)$.

Proof Since we have a homogeneous Markov process, the Chapman-Kolmogorov equation for a time $t+\Delta t$ gives

$$P(x_0|x,t+\Delta t) = \int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t)\, P(y|x,\Delta t). \tag{3.4}$$

We want to derive a differential equation for $P(x_0|x,t)$. Therefore we should consider $P(y|x,\Delta t)$ for an infinitesimal time Δt and apply the conditions (i)-(iii). Let $\phi(x)$ be a bump function, then multiplying (3.4) by $\phi(x)$ and integrating over x yields

$$\int_{\mathbb{R}} \mathrm{d}x\, P(x_0|x,t+\Delta t)\phi(x) = \int_{\mathbb{R}} \mathrm{d}y \int_{\mathbb{R}} \mathrm{d}x\, P(x_0|y,t)P(y|x,\Delta t)\phi(x). \tag{3.5}$$

Using the fact that x on the left-hand side is a dummy variable, we can rewrite $x\to y$ so that

$$\int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t+\Delta t)\phi(y) = \int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t) \int_{\mathbb{R}} \mathrm{d}x\, P(y|x,\Delta t)\phi(x). \tag{3.6}$$

Given that Δt is infinitesimal and that $\lim_{\Delta t\to 0} P(y|x,\Delta t)=\delta(x-y)$, the only values x that contribute to the last integral are those in the vicinity of y. Therefore we can expand $\phi(x)$ around $x=y$, so that

$$\begin{aligned}
\int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t+\Delta t)\phi(y) &\overset{\Delta t\sim 0}{\simeq} \int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t) \int_{\mathbb{R}} \mathrm{d}x\, P(y|x,\Delta t)\times\\
&\quad\times\left(\phi(y)+(x-y)\phi'(y)+\frac{1}{2}(x-y)^2\phi''(y)+\mathcal{O}\left((x-y)^3\right)\right)\\
&\overset{\Delta t\sim 0}{\simeq} \int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t)\Big(\phi(y)+\phi'(y)a(y)\Delta t+\frac{1}{2}\phi''(y)b(y)\Delta t\\
&\qquad +\mathcal{O}((\Delta t)^{\alpha})\Big).
\end{aligned} \tag{3.7}$$

In the last step we used the conditions (i) to (iii) of page 44 with $x_0 = y$. By rearranging the terms of (3.7) and taking the limit $\Delta t \to 0$ one obtains

$$\underbrace{\frac{1}{\Delta t}\int_{\mathbb{R}} \mathrm{d}y\, \phi(y)(P(x_0|y,t+\Delta t) - P(x_0 y,t))}_{\overset{\Delta t\to 0}{=} \int_{\mathbb{R}} \mathrm{d}y\, \phi(y)\frac{\partial}{\partial t}P(x_0|y,t)} = \int_{\mathbb{R}} \mathrm{d}y\, P(x_0|y,t)\left(\phi'(y)a(y) + \frac{1}{2}\phi''(y)b(y)\right). \tag{3.8}$$

Finally, integration by parts yields

$$\int_{\mathbb{R}} \mathrm{d}y\, \phi(y)\frac{\partial}{\partial t}P(x_0|y,t) = \int_{\mathbb{R}} \mathrm{d}y\, \phi(y)\left(-\frac{\partial}{\partial y}(a(y)P(x_0|y,t)) + \frac{1}{2}\frac{\partial^2}{\partial y^2}(b(y)P(x_0|y,t))\right). \tag{3.9}$$

The latter equation is valid for any function ϕ, and this completes the proof. ■

Remarks

(i) The Fokker-Planck equation is defined by the *drift function* $a(x)$ that characterizes a balistic motion, and the function $b(x) \geq 0$ that characterizes the diffusion.

(ii) The Fokker-Planck equation is said to be *linear*[2] if

$$a(x) = a_1 + a_2 x, \qquad b(x) = b, \tag{3.10}$$

and *quasilinear* if $a(x)$ is non linear and $b(x) = b$. If the equation is linear, then the solution is Gaussian.

(iii) A solution of (3.3) with initial condition $P(x_0, t_0|x, t = t_0) = \delta(x - x_0)$ is called *fundamental solution*, and defines the transition probability of a diffusive Markov process. To fully determine the process, we should find $W(x,t)$. By linearity of the Fokker-Planck equation,

$$P(x,t) = \int_{\mathbb{R}} \mathrm{d}x_0\, W(x_0,t_0)P(x_0,t_0|x,t) \tag{3.11}$$

is also solution, where $W(x_0,t_0)$ is a *distribution of initial conditions*. We have

$$P(x,t)|_{t=t_0} = W(x,t_0). \tag{3.12}$$

From now on, we will omit the initial condition in equation (3.3).

(iv) The distribution $P_s(x,t)$ is *stationary* if $\frac{\partial}{\partial t}P_s(x,t) = 0$. A stationary distribution (as far as it exists) is then a solution of

$$\frac{1}{2}\frac{\partial}{\partial x}(b(x)P_s(x)) = a(x)P_s(x). \tag{3.13}$$

(v) The distribution *approaches the stationary distribution* over time if

$$\lim_{t\to\infty} P(x,t) = P_s(x). \tag{3.14}$$

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[2] In the sense of the properties of $a(x)$ and $b(x)$. The Fokker-Planck equation is always linear fo P.

3.2 Wiener and Ornstein-Uhlenbeck processes

The two processes that we will consider are particular cases of the Fokker-Planck equation corresponding to some definition of $a(x)$ and $b(x)$.

3.2.1 Brownian motion (Wiener process)

The particular case $a = 0$ and $b = 2D$, $D = (\beta m\gamma)^{-1}$, in (3.3) leads to the diffusion equation (1.17). The corresponding Markov process is defined by

$$P(x_1, t_1|x_2, t_2) = \frac{1}{\sqrt{4\pi D(t_2 - t_1)}} \mathrm{e}^{-\frac{(x_2-x_1)^2}{4D(t_2-t_1)}}, \qquad t_2 > t_1, \tag{3.15}$$

$$W(x, t) = \frac{1}{\sqrt{4\pi Dt}} \mathrm{e}^{-\frac{x^2}{4Dt}}, \qquad t > 0. \tag{3.16}$$

This process is called *Wiener process*. It is homogeneous (but non-stationary), Gaussian and has zero average. Its realizations are Brownian trajectories starting from the origin.

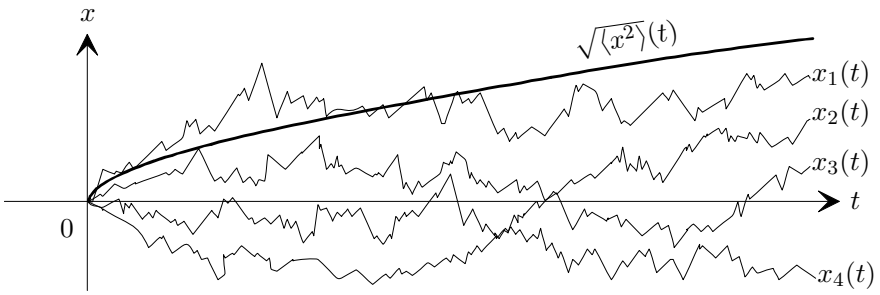

Figure 3.1: Realizations of the Wiener process and Brownian trajectories. The bold curve represents $\sqrt{\langle x^2 \rangle}(t) = \sqrt{2Dt}$, characteristic behaviour of a diffusive process.

We can check explicitely that the Wiener process defined by (3.15) and (3.16) satisfies the Chapman-Kolmogorov compatibility relations (2.41) and (2.42).

The covariance of the Wiener process is given by

$$C(t_1, t_2) = \langle x(t_1)x(t_2) \rangle = 2D \min(t_1, t_2). \tag{3.17}$$

The latter equation can be verified by calculating for $t_2 > t_1$

$$\begin{aligned}
\langle x(t_1)x(t_2) \rangle &= \int_{\mathbb{R}^2} \mathrm{d}x_1 \, \mathrm{d}x_2 \; x_1 \, x_2 \quad \underbrace{W(x_1, t_1; x_2, t_2)}_{=W(x_1,t_1)P(x_1,t_1;x_2,t_2)} \\
&\overset{(3.15)}{\underset{(3.16)}{=}} \int_{\mathbb{R}} \mathrm{d}x_1 \; x_1 \, \frac{1}{\sqrt{4Dt_1}} \, \mathrm{e}^{-\frac{x_1^2}{4Dt_1}} \underbrace{\int_{\mathbb{R}} \mathrm{d}x_2 \; x_2 \, \frac{1}{\sqrt{4D(t_2 - t_1)}} \, \mathrm{e}^{-\frac{(x_2-x_1)^2}{4D(t_2-t_1)}}}_{=x_1} \\
&= \int_{\mathbb{R}} \mathrm{d}x_1 \; x_1^2 \, \frac{1}{\sqrt{4Dt_1}} \, \mathrm{e}^{-\frac{x_1^2}{4Dt_1}} \\
&\overset{(3.2)}{=} 2Dt_1.
\end{aligned} \tag{3.18}$$

As $\langle x(t_1)x(t_2) \rangle$ is a symmetric function we find (3.17) in general.

Application: random phase and spectral broadening.

We consider an electromagnetic field $\mathcal{E}(t) = \mathcal{E}_0 \mathrm{e}^{-i\omega_0 t + i\phi(t)}$ where $\phi(t)$ is a Wiener stochastic process that obeys the diffusion equation with constant D. We will show that the Fourier transform of the correlation function of the field

$$\widetilde{C}(\omega) = \int_{\mathbb{R}} \mathrm{d}t \ \mathrm{e}^{i\omega t} C(t), \tag{3.19}$$

with

$$C(t_1 - t_2) = \langle \mathcal{E}(t_1) \mathcal{E}^*(t_2) \rangle \,, \tag{3.20}$$

is equal to the Lorentzian

$$\widetilde{C}(\omega) = |\mathcal{E}_0|^2 \frac{2D}{(\omega - \omega_0)^2 + D^2}. \tag{3.21}$$

Therefore the spectral broadening is given by the diffusion coefficient D. Indeed, we have

$$\langle \mathcal{E}(t_1) \mathcal{E}(t_2)^* \rangle = |\mathcal{E}_0|^2 \mathrm{e}^{-i\omega_0 (t_1 - t_2)} \left\langle \mathrm{e}^{i(\phi(t_1) - \phi(t_2))} \right\rangle. \tag{3.22}$$

Letting $f(t) = \delta(t - t_1) - \delta(t - t_2)$, and using the fact that the generating function of the Wiener process reads

$$\left\langle \mathrm{e}^{i \int_{\mathbb{R}} \mathrm{d}t \ f(t)\phi(t)} \right\rangle = \mathrm{e}^{-D \int_{\mathbb{R}} \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}s \ f(t) f(s) \min(t,s)}, \tag{3.23}$$

we can write

$$\left\langle \mathrm{e}^{i(\phi(t_1) - \phi(t_2))} \right\rangle = \mathrm{e}^{-D(\min(t_1,t_1) - 2\min(t_1,t_2) + \min(t_2,t_2))} = \mathrm{e}^{-D|t_1 - t_2|}, \tag{3.24}$$

whose Fourier Transform is given by (3.21).

3.2.2 Ornstein-Uhlenbeck process

This process is defined by $a(v) = -\gamma v$, $b(v) = \frac{2\gamma}{\beta m} = 2\gamma^2 D$ and describes the thermalization of a particle in a fluid at termal equilibrium. The Fokker-Planck equation (3.3) gives

$$\frac{\partial}{\partial t} P(v,t) = \gamma \frac{\partial}{\partial v} (v \, P(v,t)) + \gamma^2 D \frac{\partial^2}{\partial v^2} P(v,t). \tag{3.25}$$

The corresponding Markov process is defined by the transition probability that is solution of (3.25) with $P(v_1, t_1 | v_2, t_2 = t_1) = \delta(v_2 - v_1)$,

$$P(v_1, t_1 | v_2, t_2) = \sqrt{\frac{m\beta}{2\pi}} \frac{1}{\sqrt{1 - \mathrm{e}^{-2\gamma(t_2 - t_1)}}} \exp\left[-\beta \frac{1}{2} m \frac{\left(v_2 - v_1 \mathrm{e}^{-\gamma(t_2 - t_1)} \right)^2}{1 - \mathrm{e}^{-2\gamma(t_2 - t_1)}} \right], \tag{3.26}$$

and there exists a stationary distribution, which is nothing less than the Maxwell velocity distribution

$$W(v) = \sqrt{\frac{m\beta}{2\pi}} \mathrm{e}^{-\beta \frac{1}{2} m v^2}. \tag{3.27}$$

The Ornstein-Uhlenbeck process is *stationary* and *Gaussian* with *zero average*

$$\langle v(t) \rangle = \int_{\mathbb{R}} \mathrm{d}v \ v \, W(v) = 0. \tag{3.28}$$

Once more, we can check explicitely that the distributions (3.27) and (3.28) satisfy the Chapman-Kolmogorov relations (2.41) and (2.42). By symmetry, the odd moments are zero. Let us calculate the velocity autocorrelation function. Since the process has zero average, it is the same as its covariance. Given an initial velocity $v(t_0) = v_0$, the average velocity at time t reads (according to (3.26))

$$\int_{\mathbb{R}} \mathrm{d}v \; v\, P(v_0, t_0|v, t) = v_0 \mathrm{e}^{-\gamma(t-t_0)} = \langle v \rangle_{v_0,t_0}(t), \tag{3.29}$$

hence

$$\begin{aligned}
\langle v(t_0)\, v(t) \rangle &= \int_{\mathbb{R}^2} \mathrm{d}v_0\, \mathrm{d}v \; v_0\, v \; \underbrace{W(v_0, t_0; v, t)}_{W(v_0,t_0)P(v_0,t_0|v,t)} \\
&= \int_{\mathbb{R}} \mathrm{d}v_0 \; v_0\, W(v_0) \int_{\mathbb{R}} \mathrm{d}v \; v\, P(v_0, t_0|v, t) \\
&\overset{(3.29)}{=} \int_{\mathbb{R}} \mathrm{d}v_0 \; v_0^2\, W(v_0) \mathrm{e}^{-\gamma(t-t_0)} \\
&= \frac{1}{\beta m} \mathrm{e}^{-\gamma(t-t_0)}.
\end{aligned} \tag{3.30}$$

As the process is a solution of Fokker-Planck equation, it is a stationary Gaussian Markov process. Therefore, Doob's theorem implies that its covariance must be exponential. This is confirmed by equation (3.30). Thus, the Ornstein-Uhlenbeck process (up to the choice of β, m, γ [3]) is the only process that is both stationary Gaussian and Markovian.

Let us calculate the velocity fluctuation, given an initial condition $\{v_0, t_0\}$.

$$\begin{aligned}
\left\langle v^2 \right\rangle_{v_0,t_0}(t) &= \int_{\mathbb{R}} \mathrm{d}v \; v^2\, P(v_0, t_0|v, t) \\
&= \frac{1}{\beta m} \left(1 - \mathrm{e}^{-2\gamma(t-t_0)}\right) + v_0^2 \mathrm{e}^{-2\gamma(t-t_0)}.
\end{aligned} \tag{3.31}$$

The equations (3.29) and (3.31) show that the memory of the initial condition is lost for $t \to \infty$, whereas (3.30) and (3.31) state that the fluctuations approach the value of thermal quilibrium $\frac{1}{\beta m}$. More generally, we see from (3.26) that $P(v_0, t_0|v, t)$ tends to the Maxwell distribution (3.27) as $t - t_0 \to \infty$.

3.3 Link with the Langevin equation

We note that $\langle v \rangle_{v_0,t_0}(t)$ and $\langle v^2 \rangle_{v_0,t_0}(t)$ have exactly the same value than in Langevin theory (see equations (1.82) and (1.91) of pages 17 and 18 respectively).

In what way does Langevin equation define a homogeneous Markov stochastic process?

3.3.1 White noise

To address this question, we should define the correlations of $v(t)$ from those of the random force $f(t)$. In section 1.2, we made the assumption of instantaneous correlation for the force

[3] By rescaling $\sqrt{\beta m} v = u$ we recover the notations used in the demonstration of Doob's theorem, section 2.3.2.

(1.86), without mentioning the higher-order correlations. From now on the whole process associated to $f(t)$ will be defined as Gaussian with covariance $\langle f(t_1)f(t_2)\rangle = \Gamma\,\delta(t_1-t_2)$, $\langle f\rangle(t) = 0$. Such a process with singular covariance is called *white noise*. The reason why we associate the process with white color comes from the fact that the fourier transform of $\langle f(t_1)f(t_2)\rangle$ is constant, hence all the frequencies of the spectrum have the same weight.

(i) The generating function of white noise reads

$$G(f) = \mathrm{e}^{-\frac{\Gamma}{2}\int_{\mathbb{R}}\mathrm{d}t\,|f(t)|^2}. \tag{3.32}$$

Indeed, the generating function of a Gaussian process with covariance $C(t_1,t_2)$ is

$$G(f) = \mathrm{e}^{-\frac{1}{2}\int_{\mathbb{R}^2}\mathrm{d}t_1\,\mathrm{d}t_2\;f(t_1)\,f(t_2)\,C(t_1,t_2)}, \tag{3.33}$$

Therefore, equation (3.32) follows directly from

$$C(t_1,t_2) = \Gamma\,\delta(t_1-t_2). \tag{3.34}$$

(ii) If $f(t)$ is a white noise, then $\int_0^t \mathrm{d}s\,f(s) = x(t)$ is a Wiener process. As the white noise is Gaussian and that the relation between $x(t)$ and $f(t)$ is linear, the process $x(t)$ is also Gaussian (see lemma 2.7 of page 38). Therefore it is entirely defined by its covariance

$$\langle x(t_1)x(t_2)\rangle = \Gamma\int_0^{t_1}\mathrm{d}s_1\int_0^{t_2}\mathrm{d}s_2\;\delta(s_1-s_2) = \Gamma\,\min(t_1,t_2), \tag{3.35}$$

which is identical to that of Wiener process.

(iii) The Gaussian process with covariance $\langle f(t_1)f(t_2)\rangle = \Gamma\,(t_2-t_1)$ where $\Gamma(t)$ is a rapidly decreasing function is called *colorful noise*.

Lemma 3.1 *The velocity process described by Langevin equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}v(t) = -\gamma v(t) + \sqrt{\frac{2\gamma}{\beta m}}f(t), \tag{3.36}$$

where $f(t)$ is a white noise, $\langle f(t_1)f(t_2)\rangle = \delta(t_1-t_2)$, with a thermal distribution of initial velocities is identical to the Ornstein-Uhlenbeck process.

Proof (Lemma 3.1) In Langevin equation, the relation between $v(t)$ and $f(t)$ is linear. Therefore, lemma (2.7) states that $v(t)$ is a Gaussian process. Moreover, the two processes have the same average $\langle v\rangle(t) = 0$ and the same covariance $\langle v(t_1)v(t_2)\rangle = \frac{1}{\beta m}\mathrm{e}^{-\gamma(t_2-t_1)}$. As a Gaussian process is fully determined by its covariance, we conclude that the two processes are equal. The Ornstein-Uhlenbeck process being Markovian, the velocity process described by (3.36) has the Markov property as well. ■

We see that the two descriptions given by Langevin and Fokker-Planck equations are closely related. In a physical point of view, the evolution is ruled by a general deterministic differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = F(x(t)). \tag{3.37}$$

If the system undergoes random perturbations that change much faster than the evolution of $x(t)$, it is natural to introduce a model à la Langevin by adding a white noise

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = F(x(t)) + f(t), \qquad \langle f(t_1)f(t_2)\rangle = \Gamma\,\delta(t_1 - t_2). \tag{3.38}$$

Γ has to be determined by the physics. For instance, if there is a steady state, Γ is given by its fluctuations.[4] As the solution of (3.38) is fully determined by the initial condition x_0 in t_0, any realization $f(t)$ has the Markov property (see example 1 of page 28).

We are now going to show that $x(t)$ remains Markovian after averaging $\langle\cdot\rangle_{wn}$ over the white noise realizations. For a white noise realization $f(t)$ the process distributions read

$$W_f(x_1,t_1;\ldots;x_n,t_n) = P_f(x_0,t_0|x_1,t_1)P_f(x_1,t_1|x_2,t_2)\ldots P_f(x_{n-1},t_{n-1}|x_n,t_n), \tag{3.39}$$

with $P_f(x_0,t_0|x_1,t_1) = \delta(x_1 - \phi_f(x_0,t_0;t_1))$. Here, the flow $\phi_f(x_0,t_0;t)$ depends on the action of the force between t_0 and t. The average of $W_f(x_1,t_1;\ldots;x_n,t_n)$ over the force $f(t)$ can be factorized and keeps Markov property because there isn't any correlation of the force between the consecutive time intevals $t_0 - t_1$, $t_1 - t_2$, $t_2 - t_3$, etc.

$$W(x_1,t_1;\ldots;x_n,t_n) = \langle P_f(x_0,t_0|x_1,t_1)\rangle_{wn}\,\langle P_f(x_1,t_1|x_2,t_2)\rangle_{wn}\ldots\langle P_f(x_{n-1},t_{n-1}|x_n,t_n)\rangle_{wn}\,. \tag{3.40}$$

Consequently, all the properties of the process are determined by $P(x_1,t_1|x_2,t_2) = \langle P_f(x_1,t_1|x_2,t_2)\rangle_{wn}$ which obeys Fokker-Planck equation. Moreover, as the correlations of the white noise are invariant under time translation, the averaged probabilities $\langle P_f(x_1,t_1|x_2,t_2)\rangle_{wn}$ inherit this property. Thus, *the process induced by white noise starting from equation (3.37) is homogeneous and Markovian.* The Markov property is lost if the noise is colorful.

In order to find the corresponding Fokker-Planck equation, we have to determine the drift and diffusion functions $a(x)$ and $b(x)$. To do so, we use equation (3.3) to calculate the moments of displacements starting from x_0 at time t_0 and we identify them to the quantities (i) to (iii) of page 44.

(i) $a(x)$. By integrating (3.38) over a small time interval $t - t_0$, we have

$$\underbrace{\int_{t_0}^{t}\mathrm{d}s\,\frac{\mathrm{d}}{\mathrm{d}s}x(s)}_{=x(t)-x_0} = \underbrace{\int_{t_0}^{t}\mathrm{d}s\,F(x(s))}_{\overset{t\sim t_0}{\simeq}F(x_0)(t-t_0)} + \int_{t_0}^{t}\mathrm{d}s\,f(s). \tag{3.41}$$

By averaging (3.41) over the white noise realizations, taking into account the fact that $F(x_0)$ is not random (x_0 is fixed) and using $\langle f\rangle_{wn} = 0$, we find

$$\langle x(t) - x_0\rangle_{wn} \simeq F(x_0)(t - t_0) + \int_{t_0}^{t}\mathrm{d}s\,\underbrace{\langle f\rangle\,(s)}_{=0}, \tag{3.42}$$

hence

$$a(x_0) = F(x_0). \tag{3.43}$$

[4] The Γ coefficient that measures the white noise amplitude can be inserted in the covariance as in (3.37), or in the differential equation by substituting $f(t) \to \sqrt{\Gamma}f(t)$ as in (3.36).

(ii) $b(y)$. In the same manner we have

$$\begin{aligned}\Big\langle (x(t)-x_0)^2 \Big\rangle_{wn} &= \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{t} \mathrm{d}s_2 \Big\langle \big(F(x(s_1))+f(s_1)\big)\big(F(x(s_2))+f(s_2)\big)\Big\rangle \\ &\overset{t\sim t_0}{\simeq} F(x_0)^2(t-t_0)^2 + \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{t} \mathrm{d}s_2 \underbrace{\langle f(s_1) f(s_2)\rangle}_{=\Gamma\,\delta(s_1-s_2)} \\ &= F(x_0)^2(t-t_0)^2 + \Gamma\,(t-t_0) \\ &= \Gamma(t-t_0) + \mathcal{O}\Big((t-t_0)^2\Big), \end{aligned} \tag{3.44}$$

hence

$$b(x_0) = \Gamma. \tag{3.45}$$

Thus, the corresponding Fokker-Planck equation reads

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}\big(F(x)P(x,t)\big) + \frac{\Gamma}{2}\frac{\partial^2}{\partial x^2}P(x,t). \tag{3.46}$$

Example (Smoluchowski equation for the position) A particle in a force field $F(x)$ with friction γ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}v(t) = \frac{1}{m}F(x(t)) - \gamma v(t). \tag{3.47}$$

We assume a strong friction, so that the acceleration is negligible $\frac{\mathrm{d}}{\mathrm{d}t}v(t) \sim 0$ in comparison with the other terms. Adding a white noise $f(t)$, this equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = \frac{F(x(t))}{m\gamma} + f(t). \tag{3.48}$$

Applying (3.43) and (3.46), we find

$$a(x_0) = \frac{F(x_0)}{m\gamma}, \qquad b(x_0) = \Gamma, \tag{3.49}$$

which gives the following Fokker-Planck equation

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}\left(\frac{F(x)}{m\gamma}P(x,t)\right) + \frac{\Gamma}{2}\frac{\partial^2}{\partial x^2}P(x,t). \tag{3.50}$$

This is the Smoluchowski equation (1.48) that we derived when we studied the assymetric random walk. If $F(x) = -\frac{\mathrm{d}}{\mathrm{d}x}V(x)$, we have the stationary state $P_s(x)$ determined by

$$\frac{\Gamma}{2}\frac{\partial}{\partial x}P_s(x) = -\frac{1}{m\gamma}\left(\frac{\mathrm{d}}{\mathrm{d}x}V(x)\right)P_s(x), \tag{3.51}$$

with solution

$$P_s(x) = C\,\mathrm{e}^{-\frac{2}{\Gamma m\gamma}V(x)}, \tag{3.52}$$

C being a normalization constant. In order to have thermal equilibrium $P_e(x) = C\,\mathrm{e}^{-\beta V(x)}$, we must set $\frac{2}{\Gamma\gamma m} = \beta$, which leads to the Einstein equation $D = \frac{\Gamma}{2} = \frac{1}{\beta m\gamma}$. $\diamond$

3.4 Multivariate Fokker-Planck equation

Consider a vectorial stochastic Markov process with n homogeneous components, $\mathbf{x}(t) = (x_1(t), \dots, x_n(t))$. We assume that the n variables of the process satisfy similar conditions that definition 3.1

$$\int_{\mathbb{R}^n} \mathrm{d}^3\mathbf{x}\ (x - x_0)_i\, P(\mathbf{x}_0|\mathbf{x}, t) = a_i(\mathbf{x}_0)\, t + \mathcal{O}(t^\alpha), \qquad \alpha > 1, \tag{3.53}$$

$$\int_{\mathbb{R}^n} \mathrm{d}^3\mathbf{x}\ (x - x_0)_i (x - x_0)_j\, P(\mathbf{x}_0|\mathbf{x}, t) = b_{ij}(\mathbf{x}_0)\, t + \mathcal{O}(t^\alpha), \qquad \alpha > 1, \tag{3.54}$$

with $\mathbf{a} \in \mathbb{R}^n$ is the drift vector and $\boldsymbol{b} \in M_n(\mathbb{R})$ is the $n \times n$ symmetric real $b_{ij} = b_{ji} \in \mathbb{R}$ diffusion matrix. The associated multivariate Fokker-Planck equation (without writing the initial conditions) reads

$$\boxed{\frac{\partial}{\partial t} P(\mathbf{x}, t) = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}\big(a_i(\mathbf{x}) P(\mathbf{x}, t)\big) + \frac{1}{2} \sum_{i,j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j}\big(b_{ij}(\mathbf{x}) P(\mathbf{x}, t)\big).} \tag{3.55}$$

Its derivation is the generalization of the scalar case (3.3).

3.4.1 Kramers equation

The Kramers equation (a particular case of Fokker-Planck equation (3.55)) describes the random motion of a particle in phase space. The process $\{\mathbf{x}(t), \mathbf{v}(t)\}$ is vectorial. For simplicity we will restrict ourselves to a one-dimensional space, so that the process $\{x(t), v(t)\}$ has two components. The study of Kramers equation generalizes the analysis of Brownian motion and Langevin equation in the sense that the latter dealt only with position $x(t)$ and velocity $v(t)$, respectively. We start from the equations of motion in a force field $F(x)$ with friction γ and white noise $f(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = v(t), \tag{3.56}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} v(t) = -\gamma v(t) + \frac{F(x(t))}{m} + \sqrt{\frac{2\gamma}{\beta m}} f(t). \tag{3.57}$$

To derive the corresponding Fokker-Planck equation, called *Kramers equation*, we have to find the functions

$$\mathbf{a}(x, v) = \begin{pmatrix} a_x(x, v) \\ a_v(x, v) \end{pmatrix}, \tag{3.58}$$

and

$$\boldsymbol{b}(x, v) = \begin{pmatrix} b_{xx}(x, v) & b_{xv}(x, v) \\ b_{vx}(x, v) & b_{vv}(x, v) \end{pmatrix}, \tag{3.59}$$

with $b_{xv}(x, v) = b_{vx}(x, v)$. Using the method of page 50 we have for $t \to t_0$

$$\begin{array}{lll}
\langle (x(t) - x_0) \rangle_{bb} & \simeq v_0(t - t_0) & \Longrightarrow a_x(x_0, v_0) = v_0 \\
\langle (v(t) - v_0) \rangle_{bb} & \simeq \left(-\gamma v_0 + \frac{F(x_0)}{m}\right)(t - t_0) & \Longrightarrow a_v(x_0, v_0) = -\gamma v_0 + \frac{F(x_0)}{m} \\
\langle (x(t) - x_0)^2 \rangle_{bb} & \simeq (v_0(t - t_0))^2 = \mathcal{O}\left((t - t_0)^2\right) & \Longrightarrow b_{xx}(x_0, v_0) = 0 \\
\langle (x(t) - x_0)(v(t) - v_0) \rangle_{bb} & \simeq v_0 \left(-\gamma v_0 + \frac{F(x_0)}{m}\right)(t - t_0)^2 & \Longrightarrow b_{xv}(x_0, v_0) = b_{vx}(x_0, v_0) = 0 \\
\langle (v(t) - v_0)^2 \rangle_{bb} & \simeq \frac{2\gamma}{\beta m}(t - t_0) & \Longrightarrow b_{vv}(x_0, v_0) = \frac{2\gamma}{\beta m}.
\end{array}$$

Substituting these values in (3.55) leads to the *Kramers equation*

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}P(x,v,t) + v\frac{\partial}{\partial x}P(x,v,t) + \frac{F(x)}{m}\frac{\partial}{\partial v}P(x,v,t) \\ = \gamma\left(\frac{\partial}{\partial v}(v\,P(x,v,t)) + \frac{1}{\beta m}\frac{\partial^2}{\partial v^2}P(x,v,t)\right).\end{aligned}} \tag{3.60}$$

This equation is the starting point of many studies, e.g. the analysis of metastabilities (see section 3.5 of page 54). We introduce the *particle density*[5]

$$\rho(x,t) = \int_{\mathbb{R}} \mathrm{d}v\, P(x,v,t) \tag{3.61}$$

and the *particle current*

$$j(x,t) = \int_{\mathbb{R}} \mathrm{d}v\; v\, P(x,v,t). \tag{3.62}$$

Assuming $\lim_{v\to\pm\infty} P(x,v,t) = 0$, we can integrate (3.60) over v to obtain the *continuity equation* that links $\rho(x,t)$ and $j(x,t)$

$$\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x}j(x,t) = 0. \tag{3.63}$$

By multiplying (3.60) by v and integrating it over v, one obtains the equation satisfied by the particle current $j(x,t)$

$$\frac{\partial}{\partial t}j(x,t) + \frac{\partial}{\partial x}\int_{\mathbb{R}} \mathrm{d}v\; v^2\, P(x,v,t) + \frac{F(x)}{m}\rho(x,t) = -\gamma j(x,t). \tag{3.64}$$

Remark The Kramers equation has the structure of a *kinetic equation*

$$\frac{\partial}{\partial t}P(x,v,t) + v\frac{\partial}{\partial x}P(x,v,t) + \frac{F(x)}{m}\frac{\partial}{\partial v}P(x,v,t) = I_P(x,v,t). \tag{3.65}$$

The linear operator I_P is a *collision operator*. It contains all the effects of the collision of the particle with its environment. In our case, $I_P(x,v,t)$ takes only into account the effects of friction, that we describe phenomenologically, and the collisions, that we describe with the white noise. The Boltzmann equation will have the same structure with I_P describing the microscopic dynamic of collisions.

If $I_P(x,v,t) = 0$, the knowledge of the flow of the differential system $\dot{x}(t) = v(t)$, $m\dot{v}(t) = F(x(t))$ allows us to solve (3.65). Let $\omega = (x,v)$, $t \to \phi(\omega_0,t) = \omega(t)$ a trajectory with initial condition ω_0, and $P(\omega_0)$ a distribution of initial conditions, then the distribution at time t is defined by

$$P(\omega,t) \;=\; \int_{\mathbb{R}^2} \mathrm{d}\omega_0\, P(\omega_0)\,\delta\left(\omega - \phi(\omega_0,t)\right) \;=\; P\left(\phi^{-1}(\omega,t)\right) \tag{3.66}$$

and satisfies

$$\frac{\partial}{\partial t}P(\omega,t) + v\frac{\partial}{\partial x}P(\omega,t) + \frac{F(x)}{m}\frac{\partial}{\partial v}P(\omega,t) = 0. \tag{3.67}$$

In general, as soon as $I_P \neq 0$, the Kramers equation cannot be resolved analytically and we have to do approximations. ◇

[5]This density is normalized to 1. If we consider N independent particles and rewrite $\rho(x,t) \to N\rho(x,t)$, we can normalize it to N.

3.5 Application to the metastability

As a direct application of the Kramers model, we would like to study the lifetime of a particle located in a potential well and undergoing thermal fluctuations. Consider a particle in the potential $V(x)$ depicted in figure 3.2.

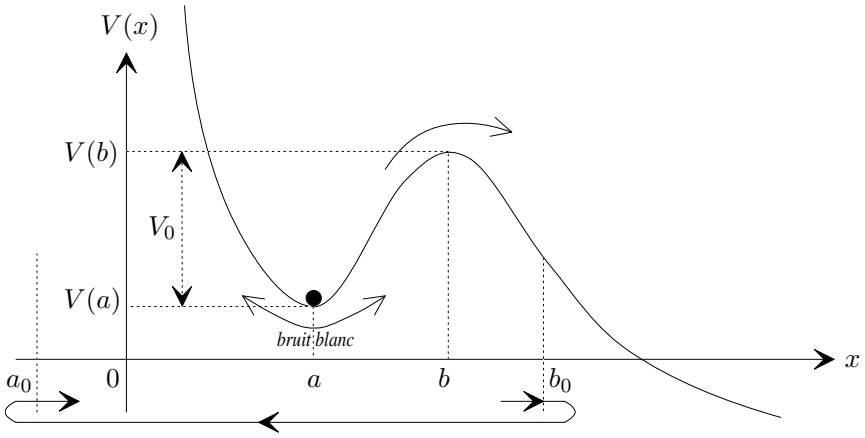

Figure 3.2: Particle fluctuating around its equilibrium position a in a potential $V(x)$ and undergoing a white noise (thermal fluctuations). Depending on the fluctuations amplitude, it can cross the potential barrier V_0 and go into region $x > b$. We simulate a steady state by introducing a pit term in b_0 that absorbs the particle and reinjects it in a source term in a_0.

Suppose first that the particle is at its equilibrium position a. Because of thermal fluctuations, it can cross the potential barrier of amplitude V_0 in b. This process is called *thermal activation*. It can describe for instance the dissociation of a molecule in a solvent of temperature T. Kramers assume that the particle is subjected to a random force $f(t)$ representing the fluctuations of the medium, therefore we must solve Kramers equations for the probability distribution. We are looking for the lifetime of a particle localized in the vicinity of a at time $t = 0$. As $F(x(t)) = -\frac{\mathrm{d}}{\mathrm{d}x}V(x(t))$, then if $f(t) = 0$ we have the deterministic equation

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}x(t) = -\frac{V'(x(t)}{m} - \gamma v(t). \tag{3.68}$$

A particle with initial condition $x_0 < a,\ v_0 = 0$ will evolve towards equilibrium position $x = a$. If we switch the random force $f(t)$ on and if thermal energy is smaller than V_0, $k_B T \ll V_0$, then the particle may get sufficient kinetic energy to cross the barrier. The case $k_B T \gg V_0$ is not of interest since the particle can freely escape the potential well. From now on, we will assume $k_B T \ll V_0$. We still have to specify the concept of lifetime, which can be defined in several ways.

In principle, we should solve (3.60) with initial distribution centered in a, and calculate the probability of finding the particle in $\{x \in [b, \infty[\}$. The lifetime can then be defined as the mean time of the first passage in $x = b$. There is no steady state in that case because the particle is not confined, and the solution of (3.60) is hard to find.

We will describe the problem from a different point of view: imagine that when the particle reaches a point $b_0 > b$, it is absorbed and reinjected with the same velocity to the left of the origin in a_0. Formally, this effect is described by adding a term $S(x, t)$ in Kramers

equation which acts as a pit in b_0, as a source in a_0, and that is zero for $x \in]a_0, b_0[$. These conditions produce a steady state and a stationary current between a_0 and b_0. We will not have to explicit $S(x,t)$ in the following as we will only focus on the properties of the steady state, $x \in [a_0, b_0]$. The absorption of the particle in b_0 leads to the boundary condition

$$P(x = b_0, v, t) = 0. \tag{3.69}$$

Besides, as the potential is confining for $x \to -\infty$, we will take $a_0 = -\infty$.

First, note that the stationary current is uniform: it follows from the continuity equation (3.63) in steady state that

$$\frac{\partial}{\partial x} j(x) = -\frac{\partial}{\partial t}\rho(x) = 0, \tag{3.70}$$

hence $j = C \in \mathbb{R}$ is constant. The lifetime is then defined as

$$\tau = \frac{1}{j}. \tag{3.71}$$

We will solve Kramers equation (3.60) in steady state and in *high friction* regime, $\gamma \gg 1$. We assume that $P(x,v)$ can be expanded in powers of γ as

$$P(x,v) \;=\; \sum_{k\geq 0} \frac{1}{\gamma^k} P^{(k)}(x,v) \;=\; P^{(0)}(x,v) + \frac{1}{\gamma} P^{(1)}(x,v) + \frac{1}{\gamma^2} P^{(2)}(x,v) + \mathcal{O}\left(\frac{1}{\gamma^3}\right), \tag{3.72}$$

such that the terms of each order satisfy (3.60). Inserting (3.72) in (3.60) yields

$$\begin{aligned} &\sum_{k\geq 0} \frac{1}{\gamma^k} \left(v \frac{\partial}{\partial x} P^{(k)}(x,v) + \frac{F(x)}{m} \frac{\partial}{\partial v} P^{(k)}(x,v) \right) \\ &\qquad = \sum_{k\geq -1} \frac{1}{\gamma^k} \left(\frac{\partial}{\partial v} \big(v\, P^{(k+1)}(x,v) \big) + \frac{1}{\beta m} \frac{\partial^2}{\partial v^2} P^{(k+1)}(x,v) \right). \end{aligned} \tag{3.73}$$

The coefficient of order γ corresponding to $k = -1$ in the right-hand side must vanish,

$$\frac{\partial}{\partial v} \left(v\, P^{(0)}(x,v) + \frac{1}{\beta m} \frac{\partial^2}{\partial v^2} P^{(0)}(x,v) \right) = 0. \tag{3.74}$$

The solution reads

$$P^{(0)}(x,v) = \varphi(v)\phi(x), \tag{3.75}$$

where

$$\varphi(v) = \sqrt{\frac{\beta m}{2\pi}} \mathrm{e}^{-\beta \frac{1}{2} m v^2} \tag{3.76}$$

is the Maxwellian and $\phi(x)$ is an unknown function of x. The equality of the $k = 0$ terms in (3.73) yields

$$\begin{aligned} \frac{\partial}{\partial v} \left(v\, P^{(1)}(x,v) + \frac{1}{\beta m} \frac{\partial}{\partial v} P^{(1)}(x,v) \right) \quad &= \quad v \frac{\partial}{\partial x} P^{(0)}(x,v) + \frac{F(x)}{m} \frac{\partial}{\partial v} P^{(0)}(x,v) \\ &\overset{(3.75)}{=} \; v \left(\frac{\partial}{\partial x}\phi(x) - \beta F(x)\phi(x) \right) \varphi(v). \end{aligned} \tag{3.77}$$

The solution of (3.77) for $P^{(1)}(x,v)$ is given by

$$P^{(1)}(x,v) = -\left(\frac{\partial}{\partial x}\phi(x) - \beta F(x)\phi(x)\right) v\varphi(v) + \psi(x)\varphi(v), \tag{3.78}$$

where $\psi(x)$ depends only on x. This follows from

$$\frac{\partial}{\partial v}\Big(v^2\varphi(v) + \underbrace{\frac{1}{\beta m}\frac{\partial}{\partial v}\left(v\varphi(v)\right)}_{=\frac{1}{\beta m}\varphi(v) - v^2\varphi(v)}\Big) \;=\; \frac{\partial}{\partial v}\left(\frac{1}{\beta m}\varphi(v)\right) \;=\; -v\varphi(v). \tag{3.79}$$

Collecting the terms, we find

$$P(x,v) = \underbrace{\phi(x)\varphi(v)}_{P^{(0)}(x,v)} + \frac{1}{\gamma}\Bigg(\underbrace{\psi(x)\varphi(v) - \left(\frac{\partial}{\partial x}\phi(x) - \beta F(x)\phi(x)\right) v\varphi(v)}_{=P^{(1)}(x,v)}\Bigg) + \mathcal{O}\left(\frac{1}{\gamma^2}\right). \tag{3.80}$$

Using $\int_{\mathbb{R}} \mathrm{d}v\, v^2\varphi(v) = \frac{1}{\beta m}$, the current reads

$$j(x) \;=\; \int_{\mathbb{R}} \mathrm{d}v\; v\, P(x,v) \;\overset{(3.80)}{=}\; -\frac{1}{\gamma}\left(\frac{1}{\beta m}\frac{\mathrm{d}}{\mathrm{d}x}\phi(x) - \frac{F(x)}{m}\phi(x)\right) + \mathcal{O}\left(\frac{1}{\gamma^2}\right). \tag{3.81}$$

As $j(x) = j$ is uniform, we can determine the function $\phi(x)$ in terms of j. Writing $F(x) = -\frac{\partial}{\partial x}V(x)$, (3.81) gives

$$\frac{\partial}{\partial x}\phi(x) + \beta\left(\frac{\partial}{\partial x}V(x)\right)\phi(x) = -\beta m\gamma j. \tag{3.82}$$

Writing $\phi(x)$ as

$$\phi(x) = \mathrm{e}^{-\beta V(x)}\mathcal{X}(x), \tag{3.83}$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{X}(x) = -\beta m\gamma j\, \mathrm{e}^{\beta V(x)}. \tag{3.84}$$

According to the boundary condition (3.69), the function $\mathcal{X}(x)$ satisfies $\mathcal{X}(b_0) = 0$ and

$$\mathcal{X}(x) = \beta m\gamma j \int_x^{b_0} \mathrm{d}x\; \mathrm{e}^{\beta V(x)}, \tag{3.85}$$

which leads to

$$\phi(x) = \beta m\gamma j\, \mathrm{e}^{-\beta V(x)} \int_x^{b_0} \mathrm{d}x\; \mathrm{e}^{\beta V(x)}. \tag{3.86}$$

Finally, the density is given by

$$\rho(x) \;=\; \int_{\mathbb{R}} \mathrm{d}v\; P(x,v) \;\overset{(3.80)}{=}\; \phi(x) + \mathcal{O}\left(\frac{1}{\gamma}\right). \tag{3.87}$$

The normalization condition $\int_{-\infty}^{b_0} \mathrm{d}x\, \rho(x) = 1$ implies at leading order

$$1 \;=\; \int_{-\infty}^{b_0} \mathrm{d}x\, \phi(x) + \mathcal{O}\left(\frac{1}{\gamma}\right) \;\overset{(3.86)}{=}\; \beta m\gamma j \int_{-\infty}^{b_0} \mathrm{d}x\; \mathrm{e}^{-\beta V(x)} \int_x^{b_0} \mathrm{d}y\; \mathrm{e}^{\beta V(y)} + \mathcal{O}\left(\frac{1}{\gamma}\right). \tag{3.88}$$

To solve these integals, we assume $k_BT \ll V_0$ such that the potential minimum in $x = a$ and maximum in $x = b$ are very narrow, and we do a parabolic approximation. The main contribution comes from a in the first integral and from b in the second one:

$$V(x) = V(a) + \frac{1}{2}V''(a)(x-a)^2 + \mathcal{O}\left(|x-a|^3\right), \tag{3.89}$$

$$V(y) = V(b) - \frac{1}{2}\left|V''(b)\right|(y-b)^2 + \mathcal{O}\left(|y-b|^3\right). \tag{3.90}$$

As the integrand is quickly decreasing, we can extend the integrals over $\mathbb{R}$, hence

$$1 = j\,\beta\,m\,\gamma\,\mathrm{e}^{\beta(V(b)-V(a))}\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{e}^{-\beta\frac{1}{2}V''(a)x^2}\int_{\mathbb{R}}\mathrm{d}y\,\mathrm{e}^{-\beta\frac{1}{2}|V''(b)|y^2} = j\,m\,\gamma\,\frac{2\pi\,\mathrm{e}^{\beta(V(b)-V(a))}}{\sqrt{V''(a)|V''(b)|}}. \tag{3.91}$$

Thus, we find the *Kramers formula*

$$\boxed{\tau = \frac{1}{j} = \frac{2\pi\,m\,\gamma\,\mathrm{e}^{\beta(V(b)-V(a))}}{\sqrt{V''(a)|V''(b)|}}.} \tag{3.92}$$

If $V''(a)$ is big, then the well is tight and the particle is close to the barrier. Therefore, the lifetime τ inside the well decreases. In the same manner, if $V''(b)$ is big, the barrier is narrow and τ also decreases. If $V(b)-V(a)$ is big, the barrier is high and τ increases. Finally, if the temperature rises, then the thermal fluctuations increase the crossing probability and the lifetime diminishes.

It should be emphasized that we have considered a classical particle. For a quantum particle, we should add the possibility of crossing the barrier by tunnel effect in the thermal activation. The competition between these two phenomena leads to an interesting problem in the quantum theory of open systems.

Using other methods, Kramers equation can also be studied in the *weak friction* regime $\gamma \ll 1$.

3.6 The laser

An interesting application of the multivariate Fokker-Planck equation is the study of the phase and the intensity of a laser beam. The evolution equation for the amplitude E of a laser mode can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}E = \underbrace{(a-c)E - b|E|^2E}_{=h(E)} + f(t), \tag{3.93}$$

where a, b, c are the *pumping*, *damping* and *interaction* coefficients, respectively. $h(E)$ contains the deterministic part of the model, which is non linear, whereas $f(t)$ is a white noise such that

$$\langle f(t)\rangle = 0, \tag{3.94}$$

$$\langle f(t_1)\,f(t_2)\rangle = 0, \tag{3.95}$$

$$\langle f(t_1)\,f(t_2)^*\rangle = D\,\delta(t_1-t_2). \tag{3.96}$$

This white noise represents the different fluctuation sources acting on the laser operation such as cavity vibration, spontaneous emission in other modes, etc.

Let us start with the deterministic part of the problem ($f(t) = 0$). We deduce the evolution equation for the luminous intensity $I = |E|^2$

$$\frac{\mathrm{d}}{\mathrm{d}t}I(t) \;=\; 2I(t)(a - c - bI(t)) \;\equiv\; F(I(t)). \tag{3.97}$$

By writing $F(I) = -\frac{\mathrm{d}}{\mathrm{d}I}V(I)$ where $V(I) = -(a-c)I^2 + \frac{2b}{3}I^3$ acts as a potential, we find the stable equilibrium points corresponding to the minima of $V(I)$, i.e.

- below threshold $a \leq c$: $I_0 = 0$,

- above threshold $a > c$: $I_0 = \frac{a-c}{b} > 0$.

If there is some white noise, the probability distribution $P(E, E^*, t)$ (considering E and E^* as independent variables) of the amplitude satisfies the Fokker-Planck equation

$$\frac{\partial}{\partial t}P = -\frac{\partial}{\partial E}\left(h(E)P\right) - \frac{\partial}{\partial E^*}\left(h^*(E)P\right) + D\frac{\partial^2}{\partial E \partial E^*}P. \tag{3.98}$$

Indeed, in our case the Fokker-Planck equation (3.55) reads

$$\frac{\partial}{\partial t}P = -\frac{\partial}{\partial E}\left(a_E P\right) - \frac{\partial}{\partial E^*}\left(a_{E^*}P\right) + \frac{1}{2}\frac{\partial^2}{\partial E^2}\left(b_E P\right) + \frac{1}{2}\frac{\partial^2}{\partial E^{*2}}\left(b_{E^*}P\right) + \frac{1}{2}\frac{\partial^2}{\partial E \partial E^*}\left(b_{EE^*}P\right), \tag{3.99}$$

where a_E, a_{E^*}, b_E, b_{E^*} and b_{EE^*} are the drift vector and diffusion matrix components. The latter are found using the method of page 50. Let us write $\Delta E = E(\Delta t) - E_0$ and $\Delta E^* = E^*(\Delta t) - E_0^*$, where E_0 is the initial condition.

(i) a_E:

$$\begin{aligned}
\langle \Delta E \rangle_{bb} &= \left\langle \int_0^{\Delta t} \mathrm{d}s \;\left(h(E) + f(s)\right) \right\rangle \\
&= \int_0^{\Delta t} \mathrm{d}s \; h(E) + \int_0^{\Delta t} \mathrm{d}s \; \underbrace{\langle f(s) \rangle}_{\overset{(3.94)}{=} 0} \\
&\overset{\Delta t \sim 0}{\simeq} \underbrace{h(E_0)}_{= a_E} \Delta t
\end{aligned} \tag{3.100}$$

(ii) a_{E^*}:

$$\langle \Delta E^* \rangle_{bb} \;=\; \left\langle \int_0^{\Delta t} \mathrm{d}s \;\left(h(E^*) + f^*(s)\right) \right\rangle \;\overset{\Delta t \sim 0}{\simeq}\; \underbrace{h(E_0^*)}_{= a_{E^*}} \Delta t \tag{3.101}$$

(iii) b_E:

$$\begin{aligned}\left\langle (\Delta E)^2 \right\rangle_{bb} &= \left\langle \int_0^{\Delta t} \mathrm{d}s_1 \int_0^{\Delta t} \mathrm{d}s_2 \ \left(h(E(s_1)) + f(s_1)\right)\left(h(E(s_2)) + f(s_2)\right) \right\rangle \\ &= \int_0^{\Delta t} \mathrm{d}s_1 \int_0^{\Delta t} \mathrm{d}s_2 \ h(E(s_1))h(E(s_2)) + \int_0^{\Delta t} \mathrm{d}s_1 \int_0^{\Delta t} \mathrm{d}s_2 \ \underbrace{\langle f(s_1)f(s_2)\rangle}_{\overset{(3.95)}{=}0} \\ &\quad +2\int_0^{\Delta t} \mathrm{d}s_1 \int_0^{\Delta t} \mathrm{d}s_2 \ h(E(s_1)) \underbrace{\langle f(s_2)\rangle}_{\overset{(3.94)}{=}0} \\ &\overset{\Delta t\sim 0}{\simeq} h(E_0)h(E_0^*)(\Delta t)^2, \end{aligned} \tag{3.102}$$

hence

$$b_E = 0. \tag{3.103}$$

(iv) b_{E^*}: similarly, we find

$$b_{E^*} = 0. \tag{3.104}$$

(v) b_{EE^*}:

$$\begin{aligned}\langle \Delta E \Delta E^* \rangle_{bb} &= \left\langle \int_0^{\Delta t} \mathrm{d}s_1 \int_0^{\Delta t} \mathrm{d}s_2 \ \left(h(E(s_1)) + f(s_1)\right)\left(h^*(E(s_2)) + f^*(s_2)\right) \right\rangle \\ &\overset{\Delta t\sim 0}{\simeq} \underbrace{D}_{=b_{EE^*}} \Delta t + \mathcal{O}\left(\Delta t^2\right) \end{aligned} \tag{3.105}$$

By inserting these expressions in (3.99) we actually find the Fokker-Planck equation (3.98) of our model.

Let us write $E = E(I,\phi) = \sqrt{I}\mathrm{e}^{i\phi}$ and consider $I = EE^*$ and $\phi = \frac{i}{2}\left(\ln(E^*) - \ln(E)\right)$ as independent variables. Using the relations

$$\left\{ \begin{array}{rcl} \dfrac{\partial}{\partial E} &=& \dfrac{\partial I}{\partial E}\dfrac{\partial}{\partial I} + \dfrac{\partial \phi}{\partial E}\dfrac{\partial}{\partial \phi} \\ \dfrac{\partial}{\partial E^*} &=& \dfrac{\partial I}{\partial E^*}\dfrac{\partial}{\partial I} + \dfrac{\partial \phi}{\partial E^*}\dfrac{\partial}{\partial \phi} \end{array} \right. \tag{3.106}$$

we calculate the right-hand side terms of the Fokker-Planck equation

$$\begin{aligned}\frac{\partial}{\partial E}(h(E)P) &= P\frac{\partial}{\partial E}h(E) + h(E)\frac{\partial P}{\partial E} \\ &= \left((a-c) - 2bI\right)P + \left((a-c)I - bI^2\right)\frac{\partial}{\partial I}P - \frac{i}{2}\left((a-c) - bI\right)\frac{\partial}{\partial \phi}P \\ &= \frac{\partial}{\partial I}\left(\left[(a-c)I - bI^2\right]P\right) - \frac{i}{2}\left((a-c) - bI\right)\frac{\partial}{\partial \phi}P, \end{aligned} \tag{3.107}$$

$$\begin{aligned}\frac{\partial^2}{\partial E^* \partial E}P &= \frac{\partial}{\partial I}P + E^*\frac{\partial}{\partial E^*}\frac{\partial}{\partial I}P - \frac{i}{2E}\frac{\partial}{\partial E^*}\frac{\partial}{\partial \phi}P \\ &= \frac{\partial}{\partial I}P + I\frac{\partial^2}{\partial I^2}P + \frac{1}{4I}\frac{\partial^2}{\partial \phi^2}P. \end{aligned} \tag{3.108}$$

By inserting (3.107), its complex conjugate and (3.108) in (3.98), we find for $P(I,\phi,t)$

$$\frac{\partial}{\partial t}P = -2\frac{\partial}{\partial I}\left(\left((a-c)I - bI^2\right)P\right) + D\frac{\partial}{\partial I}\left(I\frac{\partial}{\partial I}P\right) + \frac{D}{4I}\frac{\partial^2}{\partial\phi^2}P. \tag{3.109}$$

Consider the laser intensity distribution $\overline{P}(I,t) = \int_0^{2\pi}\mathrm{d}\phi\ P(I,\phi,t)$. $\overline{P}$ satisfies equation (3.109) without the last term[6]. The stationarity equation for $\overline{P}$ is therefore

$$\frac{\partial}{\partial I}\left\{-2\left((a-c)I - bI^2\right)\overline{P} + DI\frac{\partial}{\partial I}\overline{P}\right\} = 0. \tag{3.110}$$

As $\lim_{I\to\infty}\overline{P}(I) = 0$, we have

$$\frac{D}{4}\frac{\partial}{\partial I}\overline{P} = (2(a-c) - bI)\,\overline{P}, \tag{3.111}$$

thus the stationary solution is given by

$$\overline{P}^s(I) = C\,\mathrm{e}^{\frac{2}{D}\left((a-c)I - \frac{b}{2}I^2\right)}, \tag{3.112}$$

where C is such that $\int_0^\infty \mathrm{d}I\ \overline{P}^s(I) = 1$. (3.112) can also be written as

$$\overline{P}^s(I) = C\,\mathrm{e}^{-\frac{b}{D}(I-I_0)^2}, \qquad I_0 = \frac{a-c}{b}. \tag{3.113}$$

When $a - c > 0$ (operating laser), the maximum of $\overline{P}^s(I)$ is located in $I_0 = \frac{a-c}{b}$.

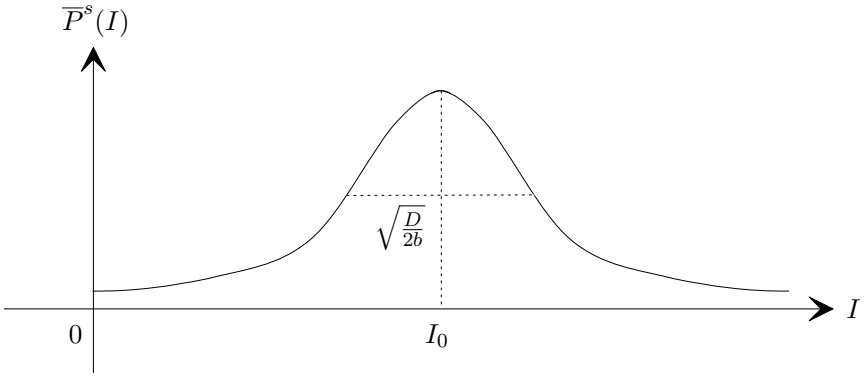

Figure 3.3: The stationary probability distribution of the laser intensity is a Gaussian centered in I_0 with width $\sqrt{\frac{D}{2b}}$.

The average intensity does not exactly coincide with to I_0:

$$\langle I\rangle_s \ = \ \int_0^\infty \mathrm{d}I\ I\,\overline{P}^s(I) \ = \ I_0 + C\int_{I_0}^\infty \mathrm{d}x\ (x - I_0)\,\mathrm{e}^{-\frac{b}{D}x^2}. \tag{3.114}$$

The correction is of order $\mathrm{e}^{-\frac{b}{D}I_0^2}$, which is very small for a weak noise (small D).

[6]We assume that $P(I,\phi,t)$ and its derivatives vanish as I tends to infinity and that $P(I,\phi,t)$ is 2π-periodic in ϕ, thus $\int_0^{2\pi}\mathrm{d}\phi\,\frac{\partial^2}{\partial\phi^2}P = 0$.

We will now study the non-stationary regime within a linear approximation. We linearize the Fokker-Planck equation (3.109) by expanding the drift term at first order in the vicinity of I_0 and by replacing the diffusion coefficients with their value in I_0. Inserting $I = I_0 + x$ in the drift term, we find at first order

$$(a-c)I - bI^2 \simeq -bI_0 x. \tag{3.115}$$

Thus, the linearized equation for $P(x,\phi,t)$ is given by

$$\frac{\partial}{\partial t}P = 2bI_0\frac{\partial}{\partial x}(xP) + DI_0\frac{\partial^2}{\partial x^2}P + \frac{D}{4I_0}\frac{\partial^2}{\partial \phi^2}P. \tag{3.116}$$

With this approximation, the evolution of $x = I - I_0$ and the phase ϕ are independent. Indeed, we can solve (3.116) for a factorized distribution $P(x,\phi,t) = P_1(x,t)P_2(\phi,t)$ with

$$\frac{\partial}{\partial t}P_1 = 2bI_0\frac{\partial}{\partial x}(xP_1) + DI_0\frac{\partial^2}{\partial x^2}P_1, \tag{3.117}$$

$$\frac{\partial}{\partial t}P_2 = \frac{D}{4I_0}\frac{\partial^2}{\partial \phi^2}P_2. \tag{3.118}$$

First of all, equation (3.117) states that $x(t) = I(t) - I_0$ is an Ornstein-Uhlenbeck process. Using the properties of this process that we have already studied, it is straightforward to show that the average intensity approaches I_0 within a relaxation time $\tau_I = \frac{1}{2bI_0} = \frac{1}{2(a-c)}$:

$$\langle I(t) - I_0\rangle = \langle x(t)\rangle = \mathrm{e}^{-2bI_0 t}, \tag{3.119}$$

and the intensity correlations are given by

$$\Big\langle (I(t_1) - I_0)\,(I(t_2) - I_0)\Big\rangle = \frac{D}{2b}\,\mathrm{e}^{-2bI_0|t_2-t_1|}. \tag{3.120}$$

Secondly, equation (3.118) states that the phase undergoes a Brownian diffusion, and that its fluctuations characteristic time is given by $\tau_\phi = \frac{2I_0}{D}$:

$$\Big\langle \phi^2(t)\Big\rangle = \frac{D}{2I_0}t. \tag{3.121}$$

This linear description, where phase and intensity evolve independently, is valid if $\tau_\phi \gg \tau_I$, i.e. if $a - c \gg \frac{1}{2}\sqrt{bD}$. When the intensity reaches its stationary value (during time τ_I), the phase undergoes a Brownian diffusion. According to the result (3.21), we conclude that the spectral broadening is of order $\frac{D}{I_0}$.

3.7 Path integral

3.7.1 Brownian motion without absorption

We would like to address the problem of calculating the average of a functional $F(x(\cdot))$ of the Brownian paths. The notation $x(\cdot)$ means that F depends on the path $x(t)$ for any t. Consider the paths starting in x_0 at time t_0 and ending in x at time t. If $F(x(\cdot))$ depends on $x(t)$ only through a finite number of times $t_1, \ldots, t_n$, then it is equivalent to a function $F(x_1, \ldots, x_n)$ of n variables, and we know that its average is given by

$$\int_{\mathbb{R}^n} \mathrm{d}x_1 \ldots \mathrm{d}x_n \; P(x_0, t_0 | x_1, t_1; \ldots; x_n, t_n; x, t)\, F(x_1, \ldots, x_n). \tag{3.122}$$

The general case is treated by taking the continuous limit, in a manner equivalent to the construction of ordinary integrals. Let us divide the interval $[t_0, t]$ in $n+1$ intervals of equal lengths

$$\tau = \frac{t - t_0}{n+1}, \tag{3.123}$$

and write

$$t_k = t_0 + k\tau, \qquad k = 0, \ldots, n, \qquad t_{n+1} = t. \tag{3.124}$$

It follows from Markov property that the probability of finding the path in $[x_1, x_1 + \mathrm{d}x_1\,]$ at τ, $[x_2, x_2 + \mathrm{d}x_2\,]$ at 2τ, …, $[x_n, x_n + \mathrm{d}x_n\,]$ at $n\tau$ can be factorized as

$$P(x_0, t_0 | x_1, t_1; \ldots; x_n, t_n; x, t)\, \mathrm{d}x_1 \ldots \mathrm{d}x_n \; = P(x_0, t_0 | x_1, t_1) \ldots P(x_n, t_n | x, t)\, \mathrm{d}x_1 \ldots \mathrm{d}x_n \,. \tag{3.125}$$

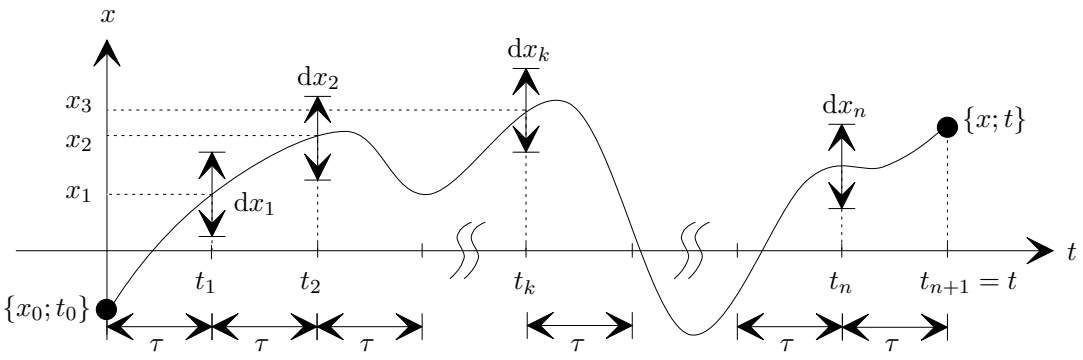

Figure 3.4: Discretization of the Brownian trajectory. The points $x_1, \ldots, x_n$ are likely to vary. Only the starting point x_0 and ending point x are fixed.

As the transition probability of the Brownian motion is given by

$$P(x_0, t_0 | x_1, t_1) = \frac{1}{\sqrt{4\pi D(t_2 - t_1)}} \mathrm{e}^{-\frac{(x_2 - x_1)^2}{4D(t_2 - t_1)}}, \tag{3.126}$$

equation (3.125) becomes

$$P(x_0, t_0 | x_1, t_1; \ldots; x_n, t_n; x, t)\, \mathrm{d}x_1 \ldots \mathrm{d}x_n \; = \left(\frac{1}{4\pi D\tau}\right)^{\frac{n+1}{2}} \mathrm{e}^{-\frac{1}{4D}\frac{1}{\tau}\sum_{k=0}^{n}(x_{k+1} - x_k)^2}\, \mathrm{d}x_1 \ldots \mathrm{d}x_n \,. \tag{3.127}$$

Note that in the limit $\tau \to 0$ the sum in the exponential tends formally to and integral

$$\lim_{\tau\to 0} \frac{1}{\tau} \sum_{k=0}^{n} (x_{k+1} - x_k)^2 = \lim_{\tau\to 0} \tau \sum_{k=0}^{n} \underbrace{\left(\frac{x(t_0 + (k+1)\tau) - x(t_0 + k\tau)}{\tau} \right)^2}_{\overset{\tau\to 0}{=} \left(\frac{\mathrm{d}}{\mathrm{d}t'} x(t')\right)^2_{t'=k\tau}}$$
$$= \int_{t_0}^{t} \mathrm{d}t' \left(\frac{\mathrm{d}}{\mathrm{d}t'} x(t') \right)^2 . \tag{3.128}$$

We define the *weight of a path* as the limit of (3.127) as $\tau \to 0$ (or equivalently as $n \to \infty$)

$$\boxed{\lim_{n\to\infty} P(x_0, t_0 | x_1, t_1; \ldots; x_n, t_n; x, t)\, \mathrm{d}x_1 \ldots \mathrm{d}x_n = \mathrm{D}\left[x(\cdot)\right] \mathrm{e}^{-\frac{1}{4D}\int_{t_0}^{t} \mathrm{d}t' \left(\frac{\mathrm{d}}{\mathrm{d}t'} x(t')\right)^2} \doteq \mathrm{d}W\,.} \tag{3.129}$$

In relation (3.129),

$$\lim_{n\to\infty} \left(\frac{1}{4\pi D\tau} \right)^{\frac{n+1}{2}} \mathrm{d}x_1 \ldots \mathrm{d}x_n = \mathrm{D}\left[x(\cdot)\right] , \tag{3.130}$$

represents the "multiple integral" over all the variables of the path. Although it is formal, the notation (3.129) is very suggestive and is commonly used by physicists. The mathematician N. Wiener (1894-1964) demonstrated that a precise mathematical definition can be given in the sense of integration theory. It is called *conditional Wiener measure* and noted $\mathrm{d}W$.

If $F(x(\cdot))$ is a functional of the paths starting at $\{x_0, t_0\}$ and ending at $\{x, t\}$, then we can write

$$\left\langle F(x(\cdot)) \right\rangle = \int_{x_0,t_0}^{x,t} \mathrm{d}W\, F(x(\cdot)). \tag{3.131}$$

The intuitive interpretation of (3.131) is that we sum over all possible paths with a weight[7] $\mathrm{e}^{-\frac{1}{4D}\int_{t_0}^{t} \mathrm{d}t' \left(\frac{\mathrm{d}}{\mathrm{d}t'} x(t')\right)^2}$. In practice, the path integral is defined by performing a discretization and taking the limit $n \to \infty$

$$\left\langle F(x(\cdot)) \right\rangle = \lim_{n\to\infty} \int_{\mathbb{R}^n} \mathrm{d}x_1 \ldots \mathrm{d}x_n\, P(x_0, t_0 | x_1, t_1, \ldots, x_n, t_n; x, t)\, F(x_1, \ldots, x_n), \tag{3.132}$$

where $F(x_1, \ldots, x_n)$ is the functional evaluated on the polygonal path such that $x_k = x(t_0 + k\tau)$.

3.7.2 Brownian motion with absorption and Feynman-Kac formula

Let us apply these concepts to the case of a Brownian motion with absorption. Assume that for a given point x, the particle has a non-zero probability $\Omega(x)$ (per unit of time) to disappear, due to a chemical reaction for instance. We are interested in computing the average survival probability $P_\Omega(x_0, t_0 | x, t)$ of the particle between times t_0 and t and the points x_0 and x. Consider first the probability that the particle will not be absorbed along a realization of the motion, with $x_k = x(t_0 + k\tau)$. For sufficiently small τ, the survival probability between t_{k-1} and t_k is given by $(1 - \tau\Omega(x_k))$, hence the statistical independence yields

[7] In fact, one can show that Brownian paths are non differentiable with probability 1 for the measure $\mathrm{d}W$. Therefore the notation (3.129) is purely formal and mnemonic. We refer to [S] for a thorough mathematical analysis.

$$\lim_{\tau\to 0}\prod_{k=0}^{n}(1-\tau\Omega(x_k)) = \lim_{\tau\to 0}\mathrm{e}^{-\tau\sum_{k=0}^{n}\Omega(x_k)} = \mathrm{e}^{-\int_{t_0}^{t}\mathrm{d}t'\,\Omega(x(t'))}, \tag{3.133}$$

where we have used $\mathrm{e}^{-\tau\Omega(x_k)} = 1-\tau\Omega(x_k)+\mathcal{O}(\tau^2)$. This functional corresponds to the probability that the particle is not absorbed for a given realization. The survival probability $P_\Omega(x_0,t_0|x,t)$ is given by the average of (3.133) over all Brownian realizations. Thus, we have to perform the average of (3.133) according to (3.132), remembering that $\tau\to 0$ is equivalent to $n\to\infty$.

$$\begin{aligned} P_\Omega(x_0,t_0|x,t) &= \lim_{n\to\infty}\int_{\mathbb{R}^n}\mathrm{d}x_1\,\ldots\mathrm{d}x_n\,P(x_0,t_0|x_1,t_1,\ldots,x_n,t_n;x,t)\mathrm{e}^{-\tau\sum_{k=0}^{n}\Omega(x_k)} \\ &\overset{(3.125)}{=} \lim_{n\to\infty}\int_{\mathbb{R}^n}\mathrm{d}x_1\,\ldots\mathrm{d}x_n\,P(x_0,t_0|x_1,t_1)\ldots P(x_n,t_n|x,t)\mathrm{e}^{-\tau\sum_{k=0}^{n}\Omega(x_k)} \end{aligned} \tag{3.134}$$

Now, we know that (see section 2.2.3)

$$P(x_0,t_0|x,t) = \langle x_0|T_{t-t_0}|x\rangle \tag{3.135}$$

is given by the matrix elements of the diffusion semigroup

$$T_{t-t_0} = \mathrm{e}^{-(t-t_0)G_0}, \tag{3.136}$$

with generator (2.58)

$$G_0 = -D\frac{\mathrm{d}^2}{\mathrm{d}x^2}. \tag{3.137}$$

Introduce the operator $\hat{\Omega}$ that simply multiplies the states $|x\rangle$ as

$$\hat{\Omega}\,|x\rangle = \Omega(x)\,|x\rangle\,. \tag{3.138}$$

The insertion of (3.138) and (3.135) in (3.134) with $t_{i+1}-t_i=\tau\ \forall\, i=0,\ldots,n$ yields

$$P_\Omega(x_0,t_0|x,t) = \lim_{n\to\infty}\int_{\mathbb{R}^n}\mathrm{d}x_1\ldots\mathrm{d}x_n\,\langle x_0|\mathrm{e}^{-\tau\hat{\Omega}}\mathrm{e}^{-\tau G_0}|x_1\rangle\langle x_1|\ldots|x_n\rangle\langle x_n|\mathrm{e}^{-\tau\hat{\Omega}}\mathrm{e}^{-\tau G_0}|x\rangle. \tag{3.139}$$

The completeness relation $\int_{\mathbb{R}}\mathrm{d}x\,|x\rangle\,\langle x| = \mathbb{1}$ that is valid for each integration over $x_1,\ldots,x_n$ leads to

$$P_\Omega(x_0,t_0|x,t) = \langle x_0|\lim_{n\to\infty}\left(\mathrm{e}^{-\frac{(t-t_0)}{n+1}\hat{\Omega}}\mathrm{e}^{-\frac{(t-t_0)}{n+1}G_0}\right)^{n+1}|x\rangle. \tag{3.140}$$

The limit inside (3.140) is calculated using the *Lie-Trotter formula.*

Theorem 3.1 (Lie-Trotter formula) *Let A and B be two linear operators (that do not necessary commute, $[A,B]\neq 0$), then*[8]

$$\lim_{n\to\infty}\left(\mathrm{e}^{\frac{A}{n}}\mathrm{e}^{\frac{B}{n}}\right)^n = \mathrm{e}^{A+B}. \tag{3.141}$$

[8]We refer to [Si] for the detailed validity conditions of the formula.

This theorem will be demonstrated below. By using (3.141) in (3.140) we finally obtain

$$P_\Omega(x_0,t_0|x,t) = \langle x_0|\mathrm{e}^{-(t-t_0)G}|x\rangle, \tag{3.142}$$

$$G = G_0 + \hat{\Omega}, \tag{3.143}$$

hence the differential equation for $P_\Omega(x_0,t_0|x,t)$ reads

$$\boxed{\begin{array}{lcl} \dfrac{\partial}{\partial t}P_\Omega(x_0,t_0|x,t) & = & D\dfrac{\partial^2}{\partial x^2}P_\Omega(x_0,t_0|x,t) - \Omega(x)P_\Omega(x_0,t_0|x,t), \\ P_\Omega(x_0,t_0|x,t=t_0) & = & \delta(x-x_0). \end{array}} \tag{3.144}$$

The particular case of Brownian motion is obtained by setting $\hat{\Omega}=0$. In the case of non-zero absorption $\Omega(x)\neq 0$, the survival probability of the particle during $t-t_0$ is given by $\int_{\mathbb{R}}\mathrm{d}x\,P_\Omega(x_0,t_0|x,t)<1$ for any ending point. Therefore, $P_\Omega(x_0,t_0|x,t)$ is no longer a normalized conditional probability.

The importance of this result is that it reduces the problem to solving a partial differential equation instead of calculating a functional integral. Reciprocally, the solution of any differential equation of the form (3.144) is given by the functional integral

$$\int_{x_0,t_0}^{x,t}\mathrm{d}W\ \mathrm{e}^{-\int_{t_0}^{t}\mathrm{d}t'\,\Omega(x(t'))}. \tag{3.145}$$

The formula (3.145) that solves (3.144) is called *Feynman-Kac formula*. In the case where the functional is not of the form (3.133), its average should be solved by the means of the general theory of Gaussian functional integrals and their perturbations.

We now show the demonstration of the Lie-Trotter formula for bounded operators. It remains valid for unbounded operators such as (2.58).

Proof (Lie-Trotter formula) Let A and B be two bounded operators, and φ the elements of the vector space in which acts A. The norm $||\cdot||$ is defined by $||A|| = \sup_{||\varphi||=1}||A\varphi||$ and satisfies the following inequalities

$$||A\,B|| \leq ||A||\,||B||, \tag{3.146}$$

$$||A+B|| \leq ||A|| + ||B||. \tag{3.147}$$

Defining

$$C = \mathrm{e}^{\frac{A+B}{n}}, \qquad D = \mathrm{e}^{\frac{A}{n}}\mathrm{e}^{\frac{B}{n}}, \tag{3.148}$$

we have to show that $\lim_{n\to\infty}||C^n - D^n|| = 0$, i.e. that the distance between $C^n = \mathrm{e}^{A+B}$ and D^n tends towards 0 as $n\to\infty$. Since A and B are bounded operators, there exist $a\in\mathbb{R}$ and $b\in\mathbb{R}$ such that

$$||A|| \leq a, \qquad ||B|| \leq b. \tag{3.149}$$

We have

$$C = \mathbb{1} + \frac{A+B}{n} + \mathcal{O}\left(\frac{1}{n^2}\right), \tag{3.150}$$

$$D = \left(\mathbb{1} + \frac{A}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)\right)\left(\mathbb{1} + \frac{B}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)\right) = \mathbb{1} + \frac{A+B}{n} + \mathcal{O}\left(\frac{1}{n^2}\right), \tag{3.151}$$

hence

$$||C - D|| = \mathcal{O}\left(\frac{1}{n^2}\right). \tag{3.152}$$

Moreover,

$$\begin{aligned}
||C|| &= \left|\left| \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{A+B}{n}\right)^k \right|\right| \\
&\overset{(3.147)}{\leq} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{||(A+B)^k||}{n^k} \\
&\overset{(3.146)}{\leq} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{||A+B||^k}{n^k} \\
&= \mathrm{e}^{\frac{||A+B||}{n}} \\
&\overset{(3.147)}{\leq} \mathrm{e}^{\frac{||A||+||B||}{n}},
\end{aligned} \tag{3.153}$$

and in the same way,

$$\begin{aligned}
||D|| &= \left|\left| \sum_{k=0}^{\infty} \frac{1}{k!} \frac{A^k}{n^k} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{B^k}{n^k} \right|\right| \\
&\overset{(3.146)}{\leq} \left|\left| \sum_{k=0}^{\infty} \frac{1}{k!} \frac{A^k}{n^k} \right|\right| \left|\left| \sum_{k=0}^{\infty} \frac{1}{k!} \frac{B^k}{n^k} \right|\right| \\
&\overset{(3.147)}{\leq} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{||A^k||}{n^k} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{||B^k||}{n^k} \\
&\overset{(3.146)}{\leq} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{||A||^k}{n^k} \sum_{k=0}^{\infty} \frac{1}{k!} \frac{||B||^k}{n^k} \\
&= \mathrm{e}^{\frac{||A||}{n}} \mathrm{e}^{\frac{||B||}{n}} \\
&= \mathrm{e}^{\frac{||A||+||B||}{n}}.
\end{aligned} \tag{3.154}$$

Thus for $n > 1$

$$\begin{aligned}
||C^n - D^n|| &= \left|\left| \sum_{k=1}^{n} C^{k-1}(C-D)D^{n-k} \right|\right| \\
&\overset{(3.147)}{\leq} \sum_{k=1}^{n} ||C^{k-1}(C-D)D^{n-k}|| \\
&\overset{(3.146)}{\leq} ||C-D|| \sum_{k=1}^{n} ||C^{k-1}||\, ||D^{n-k}|| \\
&\overset{(3.146)}{\leq} ||C-D|| \sum_{k=1}^{n} ||C||^{k-1}\, ||D||^{n-k} \\
&\overset{(3.153)}{\overset{(3.154)}{\leq}} ||C-D||\, n\, \mathrm{e}^{\frac{n-1}{n}(||A||+||B||)} \\
&\overset{(3.149)}{\leq} ||C-D||\, n\, \mathrm{e}^{\frac{n-1}{n}(a+b)}.
\end{aligned} \tag{3.155}$$

Given that $||C-D|| = \mathcal{O}\left(\frac{1}{n^2}\right)$ and that $\frac{n-1}{n} = \mathcal{O}(1)$, equation (3.155) becomes

$$||C^n - D^n|| = \mathcal{O}\left(\frac{1}{n}\right), \tag{3.156}$$

therefore $\lim_{n\to\infty} ||C^n - D^n|| = 0$, and this completes the proof. ■

Remark (Feynman integral) We note again the analogy with the quantum formalism if we identify the generator G of (3.143) to the Hamiltonian $H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ of a quantum particle in a potential $V(x)$. This analogy can be extended in terms of path integrals in quantum mechanics. In that case, one can show that the quantum propagator

$$U(t,t_0) \;=\; \mathrm{e}^{-i\frac{t-t_0}{\hbar}H} \;=\; \mathrm{e}^{i(t-t_0)\left(\frac{\hbar}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{\hbar}V(x)\right)} \tag{3.157}$$

is given by the kernel of the evolution operator (3.157)

$$\langle x|U(t,t_0)|x_0\rangle = \int_{x_0,t_0}^{x,t} \mathrm{D}\left[x(\cdot)\right]\, \mathrm{e}^{\frac{i}{\hbar}S(x(\cdot))}, \tag{3.158}$$

where

$$S\left(x(\cdot)\right) = \int_{t_0}^{t} \mathrm{d}s\, \left(\frac{1}{2}m\left(\frac{\mathrm{d}}{\mathrm{d}s}x(s)\right)^2 - V(x(s))\right) \tag{3.159}$$

is the classical action.[9] This formulation is appropriate for studying the semiclassical limit of quantum mechanics.

The quantum propagator (3.157) can be obtained by analytical continuation of the Brownian propagator (3.136)

$$T_{t-t_0} \;=\; \mathrm{e}^{-(t-t_0)G} \;=\; \mathrm{e}^{(t-t_0)\left(D\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \hat{\Omega}(x)\right)} \tag{3.160}$$

to the complex plane of time, by evaluating (3.160) on the purely imaginary time axis.

Despite theses analogies, the interpretation and the mathematics involved in Wiener and Feynman integrals are very different. One the one hand, the Wiener integral performs a Gaussian-weighted average and has a well defined mathematical meaning. The Brownian propagator describes the *irreversible* evolution of a *classical probability density*. On the other hand, the Feynman integral involves only phases and has no probabilistic interpretation. The quantum propagator describes the *reversible* evolution of a *quantum probability amplitude*.

We can say from formula (3.158) that the probability amplitude of finding a quantum particle in x at time t is given by a linear superposition of states, each contributing by a phase factor $\mathrm{e}^{\frac{i}{\hbar}S(x(\cdot))}$ corresponding to a possible classical trajectory. While the realizations of Brownian paths are in principle physically observable, this is not the case for trajectories involved in Feynman integral because of the uncertainty principle, which states that speed and position of a quantum particle cannot be simultaneously known with an arbitrary

[9] The kernel of the evolution operator given by (3.158) can be used to calculate the wave function $\psi(x,t)$ thanks to $\psi(x,t) = \langle x|\psi_t\rangle = \int_{\mathbb{R}} \mathrm{d}x_0\, \langle x|U(t,t_0)|x_0\rangle\, \langle x_0|\psi\rangle$.

precision. Calculating the quantum evolution with the functional integral (3.158) requires difficult integration of oscillating functions.

◇

3.7.3 Polymers as Brownian paths

Let us come back to the example of random molecular chain of section 1.1.6. In the continuous limit, this chain can be considered as a Brownian path $\mathbf{r}(s)$, $0 \leq s \leq N$, where $N \gg 1$ is the number of its monomers.

By using the functional integral, we can also write equation (1.78) in the form $P(\mathbf{r}) = \int_{0,0}^{\mathbf{r},N} \mathrm{d}W$, with $\mathrm{d}W$ given by (3.129). This expression allows us to deal with an external potential or to take into account the fact that two neighbour monomers cannot occupy the same position because of their mutual repulsion. In the first case, each monomer is subjected to an external potential $V(\mathbf{r})$, and in the continuous limit an infinitesimal segment $\mathbf{r}(s)$ of a polymer is subjected to the potential $V(\mathbf{r}(s))\mathrm{d}s$. Thus, at thermal equilibrium, the distribution of the chain spreading $\mathbf{r}$ is given by the functional integral (up to a normalization constant)

$$P_V(\mathbf{0}|\mathbf{r}, N) = C_N \int_{0,0}^{\mathbf{r},N} \mathrm{d}W \ \mathrm{e}^{-\beta \int_0^N \mathrm{d}s \ V(\mathbf{r}(s))} \tag{3.161}$$

which can be studied by using Feynman-Kac formula and the associated differential equation.

Absorption of polymers on a membrane

A flat membrane creates a potentiel $V(x)$ (see Fig. 3.5), where $\widehat{\mathbf{e}}_x$ is the normal direction to the membrane plane ($\mathbf{r} = (x, y, z)$):

$V(x) \to \infty$, $x \to -\infty$ (the membrane is impenetrable),

$V(x)$ forms a potential well (the membrane is attractive),

$V(x) = 0$, $x \geq x_0$ (the membrane has no effect on a large distance).

As that the associated diffusion constant is equal to $D = a^2/6$ (see section 1.1.6), it follows from (3.143) that

$$P_V(\mathbf{0}|\mathbf{r}, N) = c_N \langle \mathbf{0}|\mathrm{e}^{-N\,G}|\mathbf{r}\rangle, \tag{3.162}$$

where the generator G of the process is given by

$$G = -\frac{a^2}{6}\Delta + \beta V = -\frac{a^2}{6}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \beta V(x). \tag{3.163}$$

$P_V(\mathbf{0}|\mathbf{r}, N)$ can be written in terms of the eigenfunctions Ψ_α and eigen energies E_α of G as

$$P_V(\mathbf{0}|\mathbf{r}, N) = c_N \sum_\alpha \mathrm{e}^{-N\,E_\alpha} \Psi_\alpha(\mathbf{0})\Psi_\alpha(\mathbf{r}). \tag{3.164}$$

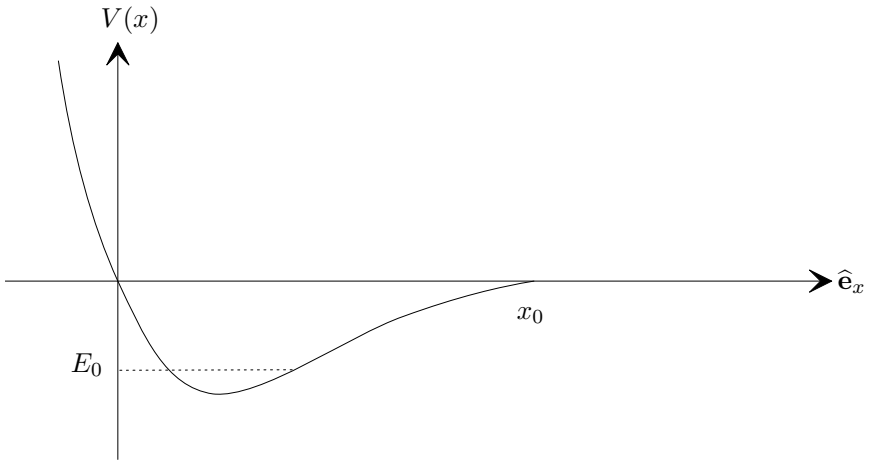

Figure 3.5: Potential of the membrane and fundamental energy E_0 of the polymer.

In order to solve the eigenvalue equation $G\Psi_\alpha = E_\alpha \Psi_\alpha$ we impose periodic boundary conditions of period L in the directions y and z. Therefore,

$$\Psi_\alpha(x,y,z) = \psi_n(x)\frac{\mathrm{e}^{ik_y y}}{\sqrt{L}}\frac{\mathrm{e}^{ik_z z}}{\sqrt{L}}, \qquad E_\alpha = \epsilon_n + \frac{6}{a^2}(k_y^2 + k_z^2), \tag{3.165}$$

where $k_y = 2\pi n_y/L$,$k_z = 2\pi n_z/L$,n_y, $n_z \in \mathbb{Z}$, are wavenumbers and ψ_n, ϵ_n, $n \in \mathbb{N}$, are the eigenstates and eigenvalues of the one-dimensional problem [10]

$$-\frac{a^2}{6}\frac{\partial^2}{\partial x^2}\psi_n(x) + \beta V(x)\psi_n(x) = \epsilon_n \psi_n(x), \qquad \epsilon_0 < \epsilon_1 \leq \epsilon_2 \leq \dots. \tag{3.166}$$

Consider the distribution $P_V(\mathbf{0}|x,0,0,N)$ of the ending point of the polymer in direction x perpendicular to the membrane for $N \gg 1$. In this limit, it is clear that the leading term of the sum (3.164) corresponds to the fundamental state $n = n_y = n_z = 0$ with energy $E_0 = \epsilon_0$:

$$\begin{aligned} P_V(\mathbf{0}|x,0,0,N) &\overset{x\to\infty}{\asymp} c_N \mathrm{e}^{-\epsilon_0 N}\Psi_0(\mathbf{0})\Psi(x,0,0) \\ &\propto d_N \psi_0(0)\psi_0(x), \end{aligned} \tag{3.167}$$

since equation (3.165) states that $\Psi_0(x,0,0)$ is proportional to the fundamental state $\psi_0(x)$ of equation (3.166) and d_N is a constant. Thus, the ending point distribution in direction x is determined by $\psi_0(x)$. As the potential vanishes for $x > x_0$ it follows from (3.166) that

$$\psi_0(x) \simeq \exp\left(-\sqrt{\frac{6|\epsilon_0|}{a^2}}x\right), \qquad x > x_0, \tag{3.168}$$

up to a normalization constant. Therefore, $a/\sqrt{6|\epsilon_0|}$ represents the typical length beyond which the probability to find the second end of a poylmer attached to the membrane becomes negligible, and provides the width of the absorbing layer.

[10] We can also impose a boundary condition for large x ($x \gg x_0$) to have an entirely discrete spectrum.

Auto-repulsive polymers

If we take the repulsion between monomers into account, the functional integral reads

$$\int_{0,0}^{\mathbf{r},N} \mathrm{d}W \ \mathrm{e}^{-\frac{\beta}{2}\int_0^N \mathrm{d}s_1 \int_0^N \mathrm{d}s_2 \ V(\mathbf{r}(s_1)-\mathbf{r}(s_2))} \tag{3.169}$$

where $V(\mathbf{r}(s_1)-\mathbf{r}(s_2))\mathrm{d}s_1\mathrm{d}s_2$ is the repulsive potential between two infinitesimal segments of the chain. With this repulsion we expect the fluctuation law for the spreading of the chain to have the form

$$\left\langle \mathbf{r}^2 \right\rangle \propto N^{2\nu}, \tag{3.170}$$

where $\nu \in [1/2, 1]$. The case $\nu = 1/2$ reflects a diffusive behaviour in which the interactions between monomers are negligible; $\nu = 1$ characterizes a polymer wherein the repulsion is so strong that it forms a rigid chain. If $\nu = 1$ the average square deviation is of the order of the number N of monomers, which means that the polymer spreads in only one dimension to form a linear chain of length Na. Let d be the space dimension, then the effects of the repulsion between monomers lead to the universal relations (excluding the volume effects)

$$\nu = \begin{cases} 1, & d = 1, \\ \frac{3}{4}, & d = 2, \\ 0.588\ldots, & d = 3, \\ \frac{1}{2}, & d > 4. \end{cases} \tag{3.171}$$

The universality stems from the fact that (3.171) does not depend on the explicit form of the potential. For dimensions greater than 4, we know that the intersection points of a Brownian path with itself form a null measurable set. Therefore a short distance repulsion does not have any effects and the exponent ν is equal to $1/2$ (we refer to [Ma] for more details).

3.8 Heavy-tailed distribution and anomalous diffusion

This section relies upon reference [Ba]. A complete review of Lévy processes and their applications in physics can be found in [Bo].

3.8.1 Brownian motion and law of large numbers

Brownian motion is characterized in that the distribution of the particle displacement $y = x_2 - x_1$ (the increment of the process) in a time step τ is given by equation (1.21)

$$P(y) = \frac{1}{\sqrt{4\pi D\tau}} \exp\left(-\frac{y^2}{4D\tau}\right). \tag{3.172}$$

The Markov property amounts to saying that the increments are independent and distributed with the same law $P(y)$. The distribution (3.172) assigns a very small probability for large increments: they are all statistically of the order of the variance $\sigma = \sqrt{2D\tau}$. Such a law with finite variance is said to have a narrow distribution. If we consider the Brownian

process $x(n)$ with dicrete time intervals $n = 0, 1, \ldots$, the probability of finding the particle (starting form the origin) in x after $n = t/\tau$ time intervals is given by

$$P(x,n) = \frac{1}{\sqrt{4\pi D n\tau}} \exp\left(-\frac{x^2}{4Dn\tau}\right), \tag{3.173}$$

which leads to the diffusive behaviour

$$\sqrt{\langle x(n)^2\rangle} = \sqrt{2D\tau n}. \tag{3.174}$$

In fact,

$$x(n) \equiv x_n = \sum_{i=1}^{n} y_n, \qquad y_i = x_{i+1} - x_i, \quad x_0 = 0, \quad x_{i+1} = x, \tag{3.175}$$

is the sum of n independent and identically distributed random variables (the n successive increments). By introducing $u_n = x_n/\sqrt{n}$, it follows from equation (3.173) that the normalized distribution of u_n is a Gaussian independent on n and a fortiori for $n \to \infty$. This is a particular case of the law of large numbers which states that the fluctuations (after rescaling $\sqrt{n}$)

$$u_n = \frac{x_n - \langle x_n\rangle}{\sqrt{n}} \tag{3.176}$$

of a sum $x_n = \sum_{i=1}^{n} y_i$ of n independent and identically distributed variables tend to a Gaussian distribution as $n \to \infty$. The theorem is valid provided that the first moment $\langle y\rangle = \int \mathrm{d}y\, yP(y)$ and second moment $\langle y^2\rangle = \int \mathrm{d}y\, y^2 P(y)$ of $P(y)$ are finite. More precisely, it is formulated as

$$\lim_{n\to\infty} \mathrm{Prob}\{u_\alpha \le u_n \le u_\beta\} = \frac{1}{\sqrt{2\pi}\sigma} \int_{u_a}^{u_b} \mathrm{d}u\, \exp\left(-\frac{u^2}{2\sigma^2}\right), \tag{3.177}$$

where $\sigma = \sqrt{\langle y^2\rangle - \langle y\rangle^2}$ is the variance of $P(y)$: it is remarkable that the limit distribution (3.177) depends only on σ and not on the explicit form of $P(y)$. The result (3.177) means that the typical realizations of the difference between the sum x_n and its average behave as

$$x_n - \langle x_n\rangle \overset{n\to\infty}{\simeq} \sqrt{n}, \tag{3.178}$$

which is in line with the diffusion law.

3.8.2 Lévy process

A process whose increments are independent and have a broad distribution describes the situations where the second moment of $P(y)$ is infinite. An example is given by Cauchy distribution

$$P(y) = \frac{2b}{\pi(y^2 + b^2)}, \qquad y \ge 0. \tag{3.179}$$

The particle has then an appreciable probability to make a considerable displacement (on the right) in a single time step. The law of large numbers is not valid anymore in its usual form and the fluctuations of the sum x_n present new properties. In particular we are out of the framework of Fokker-Planck equation as its assumptions (existence of a finite second moment, see section 3.1) are no longer valid.

Consider a positive-valued homogeneous Markov process $x(n)$ with discrete time steps $n = 0, 1, 2, \ldots$. The increments $y_n = x(n+1) - x(n)$ are positive as well[11]. The transition probability of the process is given by the increment distribution $P(y)$

$$P(x_1, n|x_2, n+1) = \begin{cases} y, & y = x_2 - x_1 \geq 0, \\ 0, & y < 0. \end{cases} \tag{3.180}$$

The probability $P(x, n)$ that the process $x(n)$ takes value x after n steps is obtained by successively using the Chapman-Kolmogorov equation

$$P(x, n) = \int_0^x \mathrm{d}x_{n-1} \ldots \int_0^{x_2} \mathrm{d}x_1 \, P(x_1) P(x_2 - x_1) \ldots P(x - x_{n-1}), \qquad x \geq 0, \tag{3.181}$$

where we have taken into account the positivity of the increments in the bounds of the integral. In order to calculate the multiple convolution in (3.181), we introduce the Laplace transform to convert it to an algebraic product,

$$\widetilde{P}(s) = \int_0^\infty \mathrm{d}y \, \mathrm{e}^{-sy} P(y), \tag{3.182}$$

$$\widetilde{P}(s, n) = \int_0^\infty \mathrm{d}x \, \mathrm{e}^{-sx} P(x, n) \overset{(3.181)}{=} \widetilde{P}(s)^n. \tag{3.183}$$

The distribution $P(y)$ will by characterized by its assymptotic behaviour

$$P(y) \overset{y \to \infty}{\simeq} \frac{b}{y^{1+\mu}}, \qquad \mu > 0. \tag{3.184}$$

If $0 < \mu \leq 2$ the second moment $\langle y^2 \rangle$ diverges and the distribution is said to be heavy-tailed (if $0 < \mu \leq 1$ the first moment diverges as well). If $\mu > 2$ the second moment is finite, the distribution is said to be narrow and the law of large numbers (3.177) is valid. The case $\mu = 1$ corresponds to the Cauchy distribution(3.179).

Even if the second moment is infinite, we can still ask a question analogous to equation (3.177): can we find a recentring a_n and a rescaling λ_n such that

$$u_n = \frac{x_n - a_n}{\lambda_n} \tag{3.185}$$

has a limit distribution for $n \to \infty$? The answer is yes, and the result for $0 < \mu < 1$ is given by

$$\lim_{n \to \infty} \mathrm{Prob}(u_\alpha \leq u_n \leq u_\beta) = \int_{u_\alpha}^{u_\beta} \mathrm{d}u \, L_{\mu,b}(u), \tag{3.186}$$

with

$$u_n = \frac{x_n}{n^{1/\mu}}, \qquad 0 < \mu < 1. \tag{3.187}$$

It is remarkable that the limit distribution $L_{\mu,b}(u)$, called Lévy law, depends only on the parameters μ and b that characterize the assymptotic behaviour (3.184) of $P(y)$. We will show below that the Laplace transform of $L_{\mu,b}(u)$ reads

$$\widetilde{L}_{\mu,b}(s) = \exp\left(-b\mu^{-1}\Gamma(1-\mu)s^\mu\right) \tag{3.188}$$

[11] We consider positive increments in order to do applications, but all these considerations can be generalized for an arbitrary increment sign.

where $\Gamma(x)$ is the Euler gamma function. It follows from (3.186) and (3.187) that the realizations of the process behave as

$$x(n) \overset{n\to\infty}{\simeq} n^{1/\mu}. \tag{3.189}$$

As $0 < \mu < 1$, its growth is much stronger than the usual diffusive process (3.174) and is also bigger than the balistic motion $x(n) \simeq n$. For instance for $\mu = 1/2$, $x(n) \simeq n^2$. As will be explained below, this comes from the fact that the individual increments can have a great amplitude.

We now give an argument that explains the behaviour (3.187) but doesn't consitute a complete proof of the theorem[12] (3.186). Consider the variable $u = x/\lambda_n$ whose normalized distribution is given by

$$Q(u,n) = \lambda_n P(\lambda_n u, n). \tag{3.190}$$

We have to show that $Q(u,n)$ has a limit for an appropriate choice of scale λ_n. Using Laplace transorms, one gets

$$\begin{aligned}
\widetilde{Q}(s,n) &= \int_0^\infty \mathrm{d}u\, \mathrm{e}^{-su} Q(u,n) \\
&= \lambda_n \int_0^\infty \mathrm{d}u\, \mathrm{e}^{-su} P(\lambda_n u, n) \\
&= \widetilde{P}\,(s/\lambda_n, n) \\
&= \left[\widetilde{P}\,(s/\lambda_n)\right]^n,
\end{aligned} \tag{3.191}$$

where we have used the change of variables $\lambda_n u = x$ and equation (3.183) in the third and last equalities. We know that the behaviour of $P(y)$ as $y \to \infty$ is given by that of $\widetilde{P}(s)$ as $s \to 0$. If the leading behaviour of $P(y)$ is of the form (3.184), then

$$\widetilde{P}(s) \overset{s\to 0}{\simeq} 1 - b\mu^{-1}\Gamma(1-\mu)s^\mu + o(s^\mu). \tag{3.192}$$

The first term comes from the normalization $\widetilde{P}(s=0) = 1$ and the second one from the Laplace transform of $y^{-(1+\mu)}$ (using the change of variable $sy \doteqdot y'$). Thus,

$$\widetilde{Q}(s,n) = \left[1 - b\mu^{-1}\Gamma(1-\mu)(s/\lambda_n)^\mu + o(s/\lambda_n)^\mu)\right]^n \tag{3.193}$$

has a limit if we choose $\lambda_n = n^{1/\mu}$:

$$\begin{aligned}
\lim_{n\to\infty} \widetilde{Q}(s,n) &= \lim_{n\to\infty} \left[1 - \frac{b\mu^{-1}\Gamma(1-\mu)s^\mu}{n} + o\left(\frac{s^\mu}{n}\right)\right]^n \\
&= \exp\left(-b\mu^{-1}\Gamma(1-\mu)s^\mu\right),
\end{aligned} \tag{3.194}$$

and we have recovered (3.188). Note that $\widetilde{L}_{\mu,b}(s) \simeq 1 - b\mu^{-1}\Gamma(1-\mu)s^\mu$, $s \to 0$, implies that the Lévy distribution $L_{\mu,b} \simeq \frac{b}{u^{1+\mu}}$, $u \to 0$, has the same decreasing (3.184) as $P(y)$. If $\mu = 1/2$ the Lévy distribution has the explicit form

$$L_{1/2,b}(u) = \frac{b}{u^{3/2}} \mathrm{e}^{-\pi b^2/u}, \qquad u \geq 0, \quad L_{1/2,b}(u) = 0, \quad u < 0. \tag{3.195}$$

[12] For more details, see [Ba, Bo] and other cited references.

A similar analysis can be done for $1 \leq \mu \leq 2$: they lead to the following anomalous diffusions:

$$\begin{aligned} x(n) &\simeq n \ln n, & \mu = 1, \\ x(n) - n\langle y \rangle &\simeq n^{1/\mu}, & 1 < \mu < 2, \\ x(n) - n\langle y \rangle &\simeq \sqrt{n \ln n}, & \mu = 2. \end{aligned} \tag{3.196}$$

We will not discuss here the corresponding Lévy distributions.

3.8.3 Lévy flights

The increments of Brownian motion (or a narrow distribution process in a general manner) have the same order of magnitude: the variance of the law. The situation is very different for heavy-tailed distributions. The probability $\mathcal{P}(\overline{y}, n)$ to observe an increment $y \geq \overline{y}$ with all other increments being smaller than $\overline{y}$ is given by

$$\mathcal{Q}(\overline{y}, n) = n\mathcal{Q}(\overline{y})(1 - \mathcal{Q}(\overline{y}))^{n-1}, \tag{3.197}$$

where

$$\mathcal{Q}(\overline{y}) = \int_{\overline{y}}^{\infty} \mathrm{d}y\, P(y) \tag{3.198}$$

is the probability to have an increment bigger than $\overline{y}$. Indeed, $\mathcal{Q}(\overline{y})(1 - \mathcal{Q}(\overline{y}))^{n-1}$ is the probability to have exactly one increment bigger than $\overline{y}$ in a sequence of n increments and the factor n takes into account that it can happen at any step of the process.

The most likely value $\overline{y}_n$ of the maximal increment is obtained by maximizing $\mathcal{Q}(\overline{y}, n)$:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\overline{y}}\mathcal{Q}(\overline{y}, n) &= n\left[(1 - \mathcal{Q}(\overline{y}))^{n-1} - (n-1)\mathcal{Q}(\overline{y})(1 - \mathcal{Q}(\overline{y}))^{n-2}\right] \frac{\mathrm{d}}{\mathrm{d}\overline{y}}\mathcal{Q}(\overline{y}) \\ &= -n\left[1 - \mathcal{Q}(\overline{y})\right]^{n-2}\left[1 - n\mathcal{Q}(\overline{y})\right] P(\overline{y}, n). \end{aligned} \tag{3.199}$$

This quantity vanishes for $1 - n\mathcal{Q}(\overline{y}) = 0$, hence

$$\int_{\overline{y}_n}^{\infty} \mathrm{d}y\, P(y) = \frac{1}{n}. \tag{3.200}$$

For Brownian motion, equation (3.172) yields

$$\frac{1}{n} = \frac{1}{\sqrt{2\pi}\sigma} \int_{\overline{y}_n}^{\infty} \mathrm{d}y \exp\left(-\frac{y^2}{2\sigma^2}\right) \overset{n\to\infty}{\simeq} \sqrt{\frac{2}{\pi}} \frac{\sigma}{y_n} \exp\left(-\frac{y_n^2}{2\sigma^2}\right), \tag{3.201}$$

hence

$$\overline{y}_n \overset{n\to\infty}{\simeq} \sigma\sqrt{2 \ln n}. \tag{3.202}$$

We see that the size of the maximal increment grows very slowly over time. Things are very different for a heavy-tailed distribution. We can estimate the order of magnitude of $\overline{y}_n$ for $n \to \infty$ by replacing $P(y)$ in equation (3.200) with its assymptotic behaviour (3.184):

$$\frac{1}{n} \simeq \int_{\overline{y}_n}^{\infty} \mathrm{d}y\, \frac{b}{y^{1+\mu}} = \frac{b}{\mu} \frac{1}{(\overline{y}_n)^{\mu}}, \tag{3.203}$$

which leads to

$$\overline{y}_n \overset{n\to\infty}{\simeq} n^{1/\mu}. \tag{3.204}$$

Comparing this result with (3.189), we see that the maximal increment has the same order of magnitude as the total displacement $x(n)$ after n steps, and the chance to observe such increment during this displacement is significant. Indeed, it follows from (3.197) and (3.200) that $\mathcal{Q}(\overline{y}, n) = (1 - 1/n)^{n-1} \simeq e^{-1} > 0$, $n \to \infty$.

Therefore, the typical motion of the particle consists essentially of a small number of displacements of amplitude proportional to $n^{1/\mu}$, called Lévy flights. It is also said that the statistics of the process is dominated by rare events. The situation is depicted in figures 3.6 and 3.7 where we have simulated a random walk in the plane, with step-lengths $y > 0$ distributed as

$$P(y) = \theta(y - y_0)\frac{\mu y_0^{\mu}}{y^{1+\mu}}. \tag{3.205}$$

The angle of an increment is equidistributed in the interval $[0, 2\pi]$. Figure 3.6 corresponds to a narrow distribution $\mu = 3$ and figure 3.7 to a heavy-tailed distribution $\mu = 3/2$.

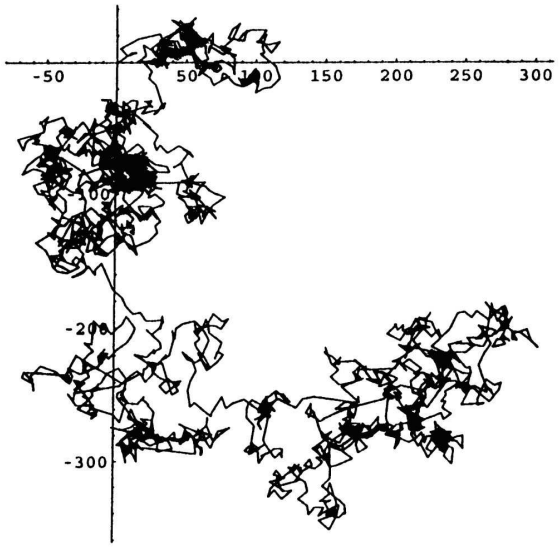

Figure 3.6: Random walk for $\mu = 3$ and $y_0 = 5$.

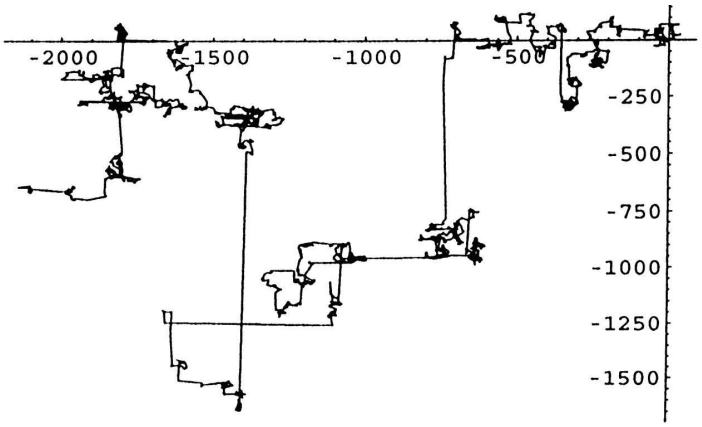

Figure 3.7: Random walk for $\mu = 3/2$ and $y_0 = 5$.

3.8.4 Applications

It was realized recently that many physical situations related to the properties of relaxation and transport should be described by heavy-tailed processes, see [Bo]. This type of process appears especially while studying the random walk of a particle in disordered media. We present here a simplified and generic model that is called Arrhenius cascade.

Arrhenius cascade

Consider a particle moving (in one dimension) in a potential $V(x)$ consisting of n wells of the same kind as 3.2 (see figure 3.8). The wells are separated by potential barriers of

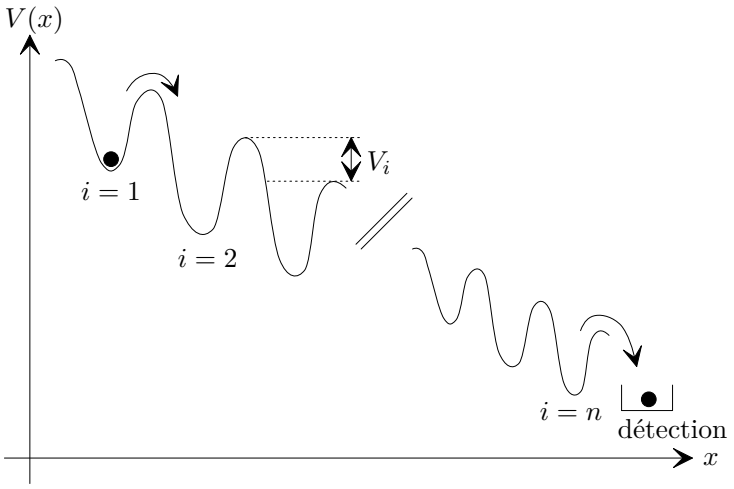

Figure 3.8: Arrhenius cascade.

amplitude $V_i > 0$. The particle undergoes an ordinary diffusion in the potential $V(x)$, ruled

by Kramers equation (see section 3.5). Thermal fluctuations carry the particle from ith to $(i+1)$th well after a mean dwell time given by (Arrhenius formula (3.92))

$$\tau_i = \tau_0 \mathrm{e}^{\beta V_i}. \tag{3.206}$$

τ_0 is a time constant that we assume to be the same for all wells [13]. If the barriers are high and the temperature is low, we can neglect the transitions where the particle crosses several wells at the same time or returns to the previous well. Thus, the overall time taken to cross n barriers is given by

$$\tau(n) = \sum_{i=1}^{n} \tau_i. \tag{3.207}$$

Let us now introduce the effect of the disordered media by stating that the barriers V_i are independent (positive) random variables distributed with the exponential law

$$F(V) = \frac{1}{E_0} \exp\left(-\frac{V}{E_0}\right), \tag{3.208}$$

where E_0 is a characteristic energy. Therefore $\tau(n)$ in equation (3.207) becomes a process with independent increments on the time axis whose steps correspond to the successive barrier crossing. The distribution $P(\tau)$ of one increment is induced by equations (3.206) and (3.208) by using $P(\tau)\mathrm{d}\tau = F(V)\mathrm{d}V$:

$$P(\tau) = F(V(\tau))\frac{\mathrm{d}}{\mathrm{d}\tau}(V(\tau)), \qquad V(\tau) = k_B T \ln\left(\tau/\tau_0\right), \quad \tau \geq \tau_0, \tag{3.209}$$

which leads to

$$P(\tau) = \mu \frac{\tau_0^{\mu}}{\tau^{1+\mu}}, \qquad \mu = \frac{k_B T}{E_0}, \quad \tau \geq \tau_0. \tag{3.210}$$

Consequently, the assymptotic behaviour of the process is ruled by the temperature T. If $k_B T > 2E_0$ we have a narrow distribution. If $k_B T \leq 2E_0$ the distribution becomes heavy-tailed, in particular $k_B T < E_0$ corresponds to the Lévy flight that we discussed in the previous sections. The overall time $\tau(n) \sim n^{E_0/k_B T}$ is not proportional to the number of crossed barriers but grows much faster. Moreover, it is realized by a small number of long stays having the same order of magnitude $n^{E_0/k_B T}$.

Laser cooling

As another example, consider the optical cooling of a gaz by photons emission and absorption. A phenomenon that prevents the atom to be at rest is the spontaneous emission. It occurs randomly and changes the atomic momentum $\mathbf{p}$ to $\mathbf{p}' = \mathbf{p} + \hbar\mathbf{k}$ where $\hbar\mathbf{k}$ is the momentum of the photon that is absorbed or emitted through an atomic transition of energy $\hbar\omega = \hbar c|\mathbf{k}|$. The resulting momentum fluctuations $\Delta p \simeq \hbar|\mathbf{k}|$ lead to an effective temperature $T_R \simeq (\Delta p)^2/2k_B m \simeq (\hbar|\mathbf{k}|)^2/2k_B m$ that appears as an absolute limit on the laser cooling. However, it is possible to overcome this limitation by carefully exploiting the properties of the interaction between atoms and photons. We refer to [Ba] for a complete description. We will confine ourselves to a brief description of how the Lévy statistics take place in this situation.

[13] In fact, because of the diffusive motion of the particle, τ_i has fluctuations but we will not consider them.

We liken the evolution of the atomic momentum to a Markovian stochastic process $p(t)$ that we assume to be one-dimensional for simplicity. The process is governed by the master equation for the probability density $\rho(p,t)$ (see equation (4.10))[14]:

$$\frac{\partial}{\partial t}\rho(p,t) = \int \mathrm{d}p' \ \left[\mathcal{W}(p'|p)\rho(p',t) - \mathcal{W}(p|p')\rho(p,t)\right]. \tag{3.211}$$

The transition rates $\mathcal{W}(p'|p)$ and $\mathcal{W}(p|p')$ have to be calculated from the quantum dynamics of the atom in interaction with photons. Let us introduce the probability $\Gamma(p)$ per unit of time to transit from state p to state $p' \neq p$

$$\Gamma(p) = \int \mathrm{d}p' \, \mathcal{W}(p|p') = \frac{1}{\tau(p)}. \tag{3.212}$$

$\Gamma(p)$ is the inverse of the lifetime of the state p. The rates have the following properties.

1. For small p and p', the transition rate from p to p' does not depend on p' and

$$\mathcal{W}(p|p') = c\Gamma(p), \qquad |p|, |p'| \leq p_0. \tag{3.213}$$

2. $\Gamma(p)$ vanishes quadratically in $p = 0$:

$$\Gamma(p) \overset{p\to 0}{\simeq} \gamma p^2, \qquad \gamma > 0. \tag{3.214}$$

This particularity plays a crucial role in the control of the quantum noise due to spontaneous emission. It can be realized physically using the properties of atom-photons interaction to create a «dark state» in which the atom cannot emmit or absorb photons.

Therefore, the vicinity of $p = 0$ can be thought of as a «trap» for the momentum. A typical realization of the process $p(t)$ is depicted in figure 3.9. $p(t)$ undergoes a random walk but if it reaches the neighbourhood $I_0 = [-p_0, p_0]$ of zero the dwell time between two steps $\tau_1, \tau_2, \tau_3, \ldots$ in this interval will be much larger than the one observed when $p(t)$ is out of this interval. This phenomenon is due to the strong suppression of the transition rate in the vicinity of $p = 0$ (equation (3.214)).

As $\Gamma(p)dt$ is the probability to leave p in the infinitesimal time $\mathrm{d}t$, the probability that $p(t)$ remains equal to p during the time τ separating two jumps is given by

$$\Pi(p,\tau) = \Gamma(p)\mathrm{e}^{-\Gamma(p)\tau}. \tag{3.215}$$

This quantity has still to be averaged over all possible realizations of the process. It is reasonable to assume that the values of p are equidistributed in I_0. The distribution of the time spent between two jumps in I_0 is then equal to

$$P(\tau) = \frac{1}{2p_0}\int_{-p_0}^{p_0} \mathrm{d}p \, \Pi(p,\tau) = \frac{1}{2p_0}\int_{-p_0}^{p_0} \mathrm{d}p \, \Gamma(p) e^{-\Gamma(p)\tau}. \tag{3.216}$$

By using quation (3.214) and performing the change of variables $u = \gamma p^2 \tau$, one obtains the assymptotic expression

$$P(\tau) \overset{\tau\to\infty}{\simeq} \frac{\gamma}{2p_0}\int_{-p_0}^{p_0} \mathrm{d}p \, p^2 e^{-\gamma p^2 \tau} \overset{\tau\to\infty}{\simeq} \frac{1}{2p_0}\sqrt{\frac{\pi}{\gamma}}\frac{1}{\tau^{3/2}}. \tag{3.217}$$

[14] Here the process is continuous and the sums are replaced by integrals.

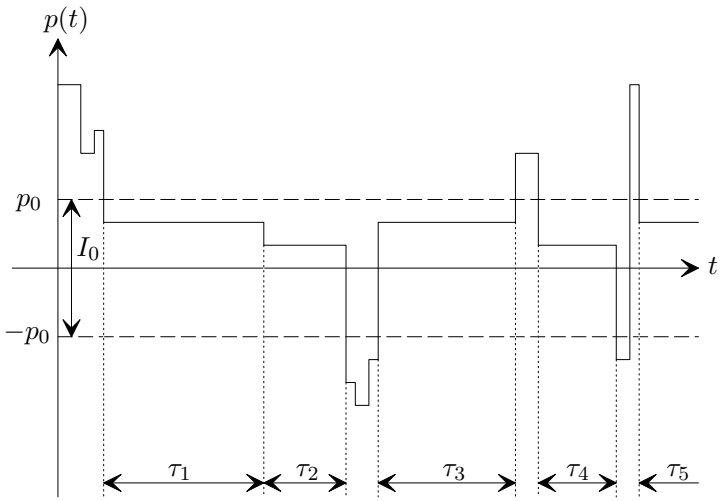

Figure 3.9: Laser cooling and statistics of the dwell time.

We see that the overall time $\tau(n) = \sum_{i=1}^{n} \tau_i$ spent in I_0 is a Lévy process whose increments are distributed with the heavy-tailed expression (3.217) corresponding to $\mu = 1/2$. We know from equation (3.189) that the total dwell time of an atom in I_0 grows as $\tau(n) \simeq n^2$. This time must still be compared to the one that $p(t)$ spends outside I_0. If the latter grows slower than n^2, we can conclude that the majority of the atoms reach the quasi-ground state $p \in I_0$ (we refer to [1] for a further discussion of these points).