Contents

Chapter 1

First passage times and escape rates

In many problems involving stochastic processes an interesting quantity to calculate is the so called *first passage time* of the process. The interest in this quantity is in its great practical applications ranging from the estimate of the swithcing time in electronic devices to theory of chemical reaction rate, adsorption on surfaces, optical bistability, polymer translocation, protein targeting a specific site in DNA, extreme value statistics in finance etc etc.

Let us first restrict ourselves to 1d stochastic processes $\{X(t)\}_{t\geq 0}$. Suppose that the process is defined on Ω with boundaries that we can denote generically as $\partial\Omega$.

If the process starts at $X(0)$ (i.e. $X(t=0)=x_0$) we can ask when it will reach *for the first time* the boundary $\partial\Omega$. This is the first passage time of the process T. Clearly, being related to a stochastic process, T is a random variables. Moreover it depends on the starting position x_0 and on the chosen boundary $\partial\omega$. To stress this point we may denote the first passage time by $T(\partial\Omega|x_0)$. Being in $d=1$ one can identify two important boundaries $\partial\Omega$:

- The boundary $\partial\Omega=[r,\xi]$ where r is a reflecting point (i.e. $j(r,t)=0$ and ξ is the value of the X for which we compute the first passage. We will see that ξ is generally taken as a absorption point (i.e. $p(x=\xi,t)=0$). Note that r can be also $-\infty$. One can also consider the opposite case $\partial\Omega=[\xi,r]$ and r can be also $+\infty$. In both cases $T=T(\partial\Omega|x_0)$ refers to the first time at which $X(t)$ reaches ξ. For example if $\partial\Omega=[r,\xi]$ we can write

$$T([r,\xi]|x_0)=\sup\{t\geq 0|X(\tau)<\xi, 0\leq\tau<t\}\,. \tag{1.1}$$

  An equivalent, maybe more intuitive, definition is

$$T([r,\xi]|x_0)=\inf\{t\geq 0|X(t)=\xi\}\,. \tag{1.2}$$

- The boundary $\partial\Omega=[\xi_L,\xi_R]$. In this case one is interested in looking at first passage time of either boundaries and we will see that, for calculation porpouses, ξ_L and ξ_R will be both absorption points of the process. The definition of $T(\partial\Omega|x_0)$ is here

$$T([\xi_L,\xi_R]|x_0)=\sup\{t\geq 0|\xi_L<X(\tau)<\xi_R, 0\leq\tau<t\}\,. \tag{1.3}$$

  or

$$T([\xi_L,\xi_R]|x_0)=\inf\{t\geq 0|X(t)=\xi_L\text{or }X(t)=\xi_R\}\,. \tag{1.4}$$

Note. In order to mantain the discussion sufficiently general we will keep, whenever possible, the notation $\partial\Omega$ and use the explicit notations $[\xi_L,\xi_R]$ or $[r,\xi]$ whenever it is required.

Probability distribution of $T(\partial\Omega|x_0)$

Since $T(\partial\Omega|x_0)$ is a random variable it is reasonable to look at its probability distribution $\mathcal{T}(\partial\Omega;t|x_0)$ defined as

$$\mathcal{T}(\partial\Omega;t|x_0) = \mathbb{P}\left\{T(\partial\Omega|x_0) < t|X(0) = x_0\right\} \tag{1.5}$$

Roughly speaking $\mathcal{T}(\partial\Omega;t|x_0)$ represents tha fraction of realizations "escaped" from the region Ω during the time interval $[0,t]$. The probability density function is then

$$p_T(\partial\Omega;t|x_0)dt = \mathbb{P}\left\{t \geq T(\partial\Omega|x_0) \geq t+dt|X(0) = x_0\right\} \equiv d\mathcal{T}(\partial\Omega;t|x_0) \tag{1.6}$$

In the case of two absorbing boundaries it is sometime convenient to consider also the conditional distribution of $T([\xi_L,\xi_R]|x_0)$ under the condition that the absorption takes place into the barrier ξ_R which we denote by $\mathcal{T}^+([\xi_L,\xi_R];t|x_0)$

$$\mathcal{T}^+([\xi_L,\xi_R];t|x_0) = \mathbb{P}\left\{T([\xi_L,\xi_R]|x_0) < t|T([\xi_L,\xi_R]|x_0) = T([-\infty,\xi_R]|x_0)\right\} \tag{1.7}$$

The quantity $\mathcal{T}^-([\xi_L,\xi_R];t|x_0)$ will denote a similar expression for the lower barrier ξ_L. Clearly

$$\mathcal{T}([\xi_L,\xi_R];t|x_0) = \mathcal{T}^+([\xi_L,\xi_R];t|x_0) + \mathcal{T}^-([\xi_L,\xi_R];t|x_0) \tag{1.8}$$

Let us call by $p_T^+([\xi_L,\xi_R];t|x_0)$ and $p_T^-([\xi_L,\xi_R];t|x_0)$ the corresponding pdf.

Survival probability

Since $\mathcal{T}(t|x_0)$ represents the fraction of "dead" realization in the interval $[0,t]$ the fraction of "survived" realization is simply $1-\mathcal{T}(t|x_0)$. We can then define the **survival probability** of the process $X(t)$ started in x_0 and with boundary $\partial\Omega$, the probability distribution

$$S(\partial\Omega;t|x_0) \equiv 1 - \mathcal{T}(\partial\Omega;(t|x_0) = \mathbb{P}\left\{T(\partial\Omega|x_0) > t|X(0) = x_0\right\} \tag{1.9}$$

Clearly

$$p_T(\partial\Omega;t|x_0)dt = d\left(1 - S(\partial\Omega;t|x_0)\right) = -dS(\partial\Omega;t|x_0) \tag{1.10}$$

Hence

$$\boxed{p_T(\partial\Omega;t|x_0)dt = -\frac{\partial}{\partial t}S(\partial\Omega;t|x_0)dt.} \tag{1.11}$$

Moments of the distribution $\mathcal{T}(t|x_0)$

In what follows let us omit, for simplicity, the explicit dependence on the boundary $\partial\Omega$. The first moment or **mean first passage time** (MFPT) is defined as

$$\mathbb{E}\left\{T(x_0)\right\} \equiv T^{(1)}(x_0) = \int_0^\infty t p_T(t|x_0)dt = -\int_0^\infty t\frac{\partial}{\partial t}S(t|x_0)dt. \tag{1.12}$$

Similarly,

$$\mathbb{E}\left\{T(x_0)^m\right\} \equiv T^{(m)}(x_0) = \int_0^\infty t^m p_T(t|x_0)dt = -\int_0^\infty t^m\frac{\partial}{\partial t}S(t|x_0)dt. \tag{1.13}$$

If we integrate the last equation by parts we get

$$T^{(m)}(x_0) = t^m S(t|x_0)\,|_0^\infty + \int_0^\infty t^{m-1}S(t|x_0)dt. \tag{1.14}$$

Since $S(0|x_0) = 1$ forall x_0 $\lim_{t\to 0} t^m S(t|x_0) = 0$. The other extreme is more delicate: clearly $S(t|x_0) \to 0$ as $t\to\infty$ but one has to see how rapidly this occurs with respect to t^m. If, for fixed m, $S(t|x_0) \sim 1/t^{m+\epsilon}$ as $t\to\infty$ we can safely assume $\lim_{t\to\infty} t^m S(t|x_0) = 0$. If this is true we finally have

$$\boxed{T^{(m)}(x_0) = m \int_0^\infty t^{m-1} S(t|x_0) dt.} \tag{1.15}$$

In particular, for the MFPT we have

$$\boxed{T^{(1)}(x_0) = \int_0^\infty S(t|x_0) dt.} \tag{1.16}$$

Relation with $p(x, t|x_0, 0)$

Given the stochastic process $X(t)$ we recall the definition of its conditional probability density $p(x, t|x_0, 0)$:

$$p(x, t|x_0, 0)dx = \mathbb{P}\left\{x \le X(t) \le x + dx | X(0) = x_0\right\}. \tag{1.17}$$

If we consider the more stringent conditional probability density

$$p_{\partial\Omega}(x, t|x_0, 0) = \mathbb{P}\left\{x \le X(t) \le x + dx, \text{without ever reached } \partial\Omega \text{ in } (0, t) | X(0) = x_0\right\} \tag{1.18}$$

it is easy to understand

$$S_{\partial\Omega}(t|x_0) = \int_\Omega p_{\partial\Omega}(x, t|x_0, 0)dx. \tag{1.19}$$

The problem is to find a way to relate $p(x, t|x_0, 0)$ with $p_{\partial\Omega}(x, t|x_0, 0)$. This is simply done by using the appropriate boundary conditions.

- In the case $\partial\Omega = [r, \xi]$ (i.e. for $T_\xi(t|x_0)$) $p_{\partial\Omega}(x, t|x_0, 0)$ is $p(x, t|x_0, 0)$ with absorbing BC in $x = \xi$ (i.e. $p(x = \xi, t|x_0, 0) = 0$) and refecting or natural in r (i.e. $j(x = r, t|x_0, 0) = 0$).
- If $\partial\Omega = [\xi_L, \xi_R]$ (i.e. for $T_{\xi_L,\xi_L}(t|x_0)$), $p_{\partial\Omega}(x, t|x_0, 0)$ is $p(x, t|x_0, 0)$ with absorbing BC in $x = \xi_L$ and $x = \xi_R$ (i.e. $p(x = \xi_L, t|x_0, 0) = p(x = \xi_L, t|x_0, 0) = 0$.

The above correspondence suggests another random variable related to first time passage problems and useful to describe extreme value statistics

Case I : $\partial\Omega = [r, \xi]$

$$Z(t|x_0) = \max\left\{X(\tau), 0 \le \tau \le t\right\}. \tag{1.20}$$

The variable $Z(t|x_0)$ gives the maximum value reached by $X(t)$ within the interval $[0, t]$ and

$$S(\xi, t|x_0) = \int_r^\xi p_{r,\xi}(x, t|x_0, 0)dx = \mathbb{P}\left\{Z(t|x_0) < \xi | X(0) = x_0\right\} \tag{1.21}$$

Clearly if we are interested in minima values we should consider $\partial\Omega = [\xi, r]$ with r that can be also $+\infty$.

Case II: $\partial\Omega = [\xi_L, \xi_R]$

If $\xi_L = -\xi_R = -\xi$ and interesting random variable is

$$Y(t|x_0) = \max\left\{|X(\tau)| < \xi, 0 \le \tau \le t\right\}. \tag{1.22}$$

and

$$S(\xi, t|x_0) = \int_{-\xi}^\xi p_{-\xi,\xi}(x, t|x_0, 0)dx = \mathbb{P}\left\{-\xi < Y(t|x_0) < \xi | X(0) = x_0\right\} \tag{1.23}$$

Note that for convenience we have moved ξ from the subscript position to stress the fact the now ξ can be seen as a variable of the problem. In other words the survival probability of the first passage time is here the probability distribution of the variables Z or Y. The relative PDF is then

$$p_s(\xi, t|x_0)d\xi = \frac{\partial}{\partial \xi} S(\xi, t|x_0)d\xi = \mathbb{P}\left\{\xi < Z(t) < \xi + d\xi | X(0) = x_0\right\} \tag{1.24}$$

As for the first passage time we can define the moments of the distribution for Z as

$$\mathbb{E}\left\{Z(t|x_0)^m\right\} \equiv Z^{(m)}(t|x_0) = \int_r^\infty \xi^m p_s(\xi, t|x_0)d\xi \tag{1.25}$$

and an integration by parts gives

$$Z^{(m)}(t|x_0) = r^m + m \int_r^\infty \xi^{m-1}(1 - S(\xi, t|x_0)d\xi \tag{1.26}$$

Similarly

$$Y^{(m)}(t|x_0) = \int_0^\infty \xi^m p_s(\xi, t|x_0) = m \int_r^\infty \xi^{m-1}(1 - S(\xi, t|x_0)d\xi \tag{1.27}$$

Unconditioned statistics

All the quantity above are conditioned to value of the initial condition x_0. To remove this condition and consider the unconditioned statistics of the problems we have to integrate over the initial distribution $p_0(x_0)$. This gives for example

$$\begin{aligned} S(\xi, t) &= \int_r^\xi S(\xi, t|x_0)p_0(x_0)dx_0 \\ &= \mathbb{P}\left\{T(\xi) > t\right\} = \mathbb{P}\left\{Z(t) < \xi\right\} \end{aligned} \tag{1.28}$$

and

$$p_T(\xi, t) = \int_r^\xi p_T(\xi, t|x_0)p_0(x_0)dx_0 = -\frac{\partial}{\partial t} S(\xi, t). \tag{1.29}$$

1.1 First passage time for continuous Gaussian Markov processes

If we restrict ourselves to continuous Gaussian Markov processes, we know that the conditioned probability density fuction of the process $p(x, t|x_0, 0)$ is a solution of the general Fokker-Planck equation

$$\frac{\partial}{\partial t} p(x, t|x_0, 0) = \frac{\partial}{\partial x}\left[-D^{(1)}(x, t)p(x, t|x_0, 0) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D^{(2)}(x, t)p(x, t|x_0, 0)\right]\right] \tag{1.30}$$

with the initial condition $p(x, t \to 0|x_0, 0) = \delta(x - x_0)$ and boundary conditions appropriate to the problem considered (see above when the relevant quantities of the first passage time problem have been introduced). We have previously seen that often it is convenient to write the FP equation in terms of the FP differential operator

$$\frac{\partial}{\partial t} p(x, t|x_0, 0) = \hat{L}_{FP}(x, t)p(x, t|x_0, 0), \tag{1.31}$$

or as continuity equation

$$\frac{\partial}{\partial t} p(x, t|x_0, 0) + \frac{\partial}{\partial x} j(x, t|x_0, 0) = 0. \tag{1.32}$$

where

$$j(x,t|x_0,0) = D^{(1)}(x,t)p(x,t|x_0,0) - \frac{1}{2}\frac{\partial}{\partial x}\left[D^{(2)}(x,t)p(x,t|x_0,0)\right] \tag{1.33}$$

is the current density. By integrating both terms of the last equation on Ω it is possible to express the mean first passage time $T^{(1)}(x_0)$ (MFPT) in term of the current density:

$$\frac{\partial}{\partial t}S(t,|x_0) = -\int_\Omega \frac{\partial}{\partial x}j(x,t|x_0,0)dx = j(x,t|x_0,0)\,|_{\partial\Omega} \tag{1.34}$$

Hence the mean first passage time can be written as

$$T^{(1)}(\partial\Omega,x_0) = -\int_0^\infty t\frac{\partial}{\partial t}S(t|x_0)dt = \int_0^\infty t\left[j(x,t|x_0,0)\,|_{\partial\Omega}\right]dt \tag{1.35}$$

A renewal equation

For continuous Markov process it is possible to write an integral equation relating the pdf $p_T([-\infty,\xi];t|x_0)$ with the conditional probability $p(x,t|x_0,t_0)$. Since the process has no memory if $x > z > x_0$ we can look at the total paths going from x_0 to x as the convolution between the paths that, starting from x_0, reach an intermediate position z within the interval $[\tau,\tau+d\tau]$ and the paths that starting at $x = z$ they will end up between $[x, d+dx]$ at time t. If we denote by $p_T(\tau|x_0)$ as the probability that the process in the interval $[\tau,\tau+d\tau]$ reaches z and by $p(x,t-\tau|z)$ as the probability of the process to be at $[x,x+dx]$ at time $t-\tau$ being started at $x = z$, we have

$$p(x,t|x_0,t_0) = \int_0^t p_T([-\infty,\xi];\tau|z)p(x,t-\tau|z,\tau)d\tau. \tag{1.36}$$

at t the process, being started at $x = x_0$ is between $[x,x+dx]$ as the sum of all the paths that starting from x_0 For the case in which $\partial\Omega = [\xi_L,\xi_L]$ we can similarly see that

$$\begin{aligned} p_T([-\infty,\xi_R];t|x_0) &= p_T^+([\xi_L,\xi_R];t|x_0) + \int_0^t p_T^-([\xi_L,\xi_R];\tau|x_0)p_T([-\infty,\xi_R];t-\tau|\xi_L)d\tau \\ p_T([\xi_L,\infty];t|x_0) &= p_T^-([\xi_L,\xi_R];t|x_0) + \int_0^t p_T^+([\xi_L,\xi_R];\tau|x_0)p_T([\xi_L,\infty];t-\tau|\xi_R)d\tau \end{aligned} \tag{1.37}$$

Hitting probability

Consider a stochastic process $X(t)$ such that $X(0) = x_0$ and that evolves within a domain $\Omega = [r,\xi]$ where r is a reflecting boundary that can be also $-\infty$. One could be interested in computing the *hitting probability* to the point ξ. According to Eq. (2.17) we can solve this problem by first computing the outgoing flux at ξ

$$j(\xi,t|x_0,0) = -D\frac{\partial p(x,t|x_0,0)}{\partial x}\,|_{x=\xi}\,. \tag{1.38}$$

The hitting probability at ξ is then given by

$$H(\xi|x_0,0) = \int_{\mathbb{R}^+} j(\xi,t|x_0,0)dt. \tag{1.39}$$

1.1.1 PDE for the evolution of $S(t|x_0)$

It is important to stress that it is not necessary to know the conditional probability $p(x,t|x_0,0)$ to compute $S(t|x_0)$. Sometimes it is more convenient to solve a PDE equation directly for $S(t|x_0)$.

In order to do that we need the **backward Fokker-Planck equation** i.e. the equation

$$\frac{\partial}{\partial t}p(x,t|x_0,0) = \hat{L}^{\dagger}_{FP}(x_0)p(x,t|x_0,0) \tag{1.40}$$

where $\hat{L}^{\dagger}_{FP}(x)$ is the adjoint of the Fokker-Planck operator. It is easy to see that in $1d$ the adjoint operator is given by

$$\hat{L}^{\dagger}_{FP}(x) = D^{(1)}(x)\frac{\partial}{\partial x} + D^{(2)}(x)\frac{\partial^2}{\partial x^2} \tag{1.41}$$

Note that we have omitted the case in which there is an explicit time dependence in $\hat{L}_{FP}$

At this point we can derive a PDE for the survival probability $S(t,|x_0)$ by simply integrating eq. (**??**) over x. This gives

$$\partial_t S(t|x_0) = \hat{L}^{\dagger}(x_0)S(t|x_0). \tag{1.42}$$

The boundary conditions depend on the kind of first passage time problem we are considering. If we consider $\partial\Omega = [r,\xi]$ then $S(t|x_0=\xi)=0$ and $\partial_{x_0}S(t|x_0)|_{x_0=r}=0$ are the correct BC. If, on the other hand, we consider $\partial\Omega = [\xi_L,\xi_R]$ the BC are $S(t|x_0=\xi_L) = S(t|x_0=\xi_R) = 0$.

1.1.2 ODE for the MFPT

To obtain a differential equation for $T^{(1)}(x_0)$ it is sufficient to integrate eq. (1.42) over all time. Indeed, since

$$\int_{\mathbb{R}^+}(\partial/\partial t)S(t|x_0) = S(\infty|x_0) - S(0|x_0) = -1, \tag{1.43}$$

one gets the following ODE for the MFPT

$$\boxed{\hat{L}^{\dagger}_{FP}(x_0)T^{(1)}(x_0) = -1.} \tag{1.44}$$

Below we will present some examples in which the above equation can be solved analytically. Since one of the most used technique involves the Laplace transform let us look at some useful realation one can get in this space.

1.1.3 Laplace transform

In many situations it is convenient to perform a Laplace transform in the time variable. For example it could be interesting to look at the Laplace transform of the pdf for the first passage time $p_T(\partial\Omega;t|x_0)$:

$$\mathcal{L}p_T(\partial\Omega;t|x_0) \equiv \hat{p}_T(\partial\Omega;s|x_0) = \int_{\mathbb{R}^+} p_T(\partial\Omega;t|x_0)e^{-st}dt. \tag{1.45}$$

Similarly we can define

$$\mathcal{L}S(\partial\Omega;t|x_0) \equiv \hat{S}_T(\partial\Omega;s|x_0) = \int_{\mathbb{R}^+} S(\partial\Omega;t|x_0)e^{-st}dt. \tag{1.46}$$

By performing a Laplace transform of equation (1.11) we get the useful relation

$$\equiv \hat{p}_T(\partial\Omega;s|x_0) = -\mathcal{L}\,[] = -s\mathcal{L}S(\partial\Omega;t|x_0) + S(\partial\Omega;t=0|x_0) = -s\hat{S}_T(\partial\Omega;s|x_0) + 1. \tag{1.47}$$

If we now take the Laplace transform of eq. (1.42) and use eq. (1.47) we get

$$\begin{aligned}\hat{p}_T(\partial\Omega;s|x_0) &= \hat{L}^{\dagger}(x_0)\mathcal{L}S(\partial\Omega;t|x_0) = \hat{L}^{\dagger}(x_0)\left(\frac{\hat{p}_T(\partial\Omega;s|x_0)-1}{s}\right)\\ &= \frac{1}{s}\hat{L}^{\dagger}(x_0)\left(1-\hat{p}_T(\partial\Omega;s|x_0)\right)\end{aligned} \tag{1.48}$$

giving

$$\boxed{\hat{L}^{\dagger}(x_0)\hat{p}_T(\partial\Omega;s|x_0) - s\hat{p}_T(\partial\Omega;s|x_0) = 0} \tag{1.49}$$

i.e. a differential equation for the Laplace transform of the pdf of the first passage time. The knowledge of $\hat{p}_T(\partial\Omega;s|x_0)$ allows also to compute the moments of the distribution. Indeed, since

$$T^{(m)}(\partial\Omega,x_0) = \int_{\mathbb{R}^+} t^m p_T(\partial\Omega;t|x_0)dt, \tag{1.50}$$

it is easy to see that

$$T^{(m)}(\partial\Omega,x_0) = (-1)^m \left(\frac{d^m\hat{p}_T}{ds^m}\right)_{s=0}. \tag{1.51}$$

In particular for the mean and the variance we have

$$T^{(1)}(\partial\Omega,x_0) = -\left(\frac{d\hat{p}_T}{ds}\right)_{s=0} \tag{1.52}$$

$$Var\left(T(\partial\Omega,x_0)\right) = \left(\frac{d^2\hat{p}_T}{ds^2}\right)_{s=0} - \left[\left(\frac{d\hat{p}_T}{ds}\right)^2_{s=0}\right]. \tag{1.53}$$

It is important to notice that if we take the Laplace tranform of the renewal equation (1.36) we get

$$\hat{p}(x,s|x_0,t_0) = \hat{p}_T([-\infty,\xi];s|x_0)\hat{p}(x,s|z) \qquad x > z > x_0. \tag{1.54}$$

The last equation suggests that $\hat{p}(x,s|x_0,t_0)$ is a function of x_0 times a function of x, say $u(x_0)u_1(x)$. Hence $\hat{p}_T([-\infty,\xi];s|x_0) = u(x_0)/u(z)$. Similarly, for $x < z < x_0$ we get $\hat{p}_T([-\infty,\xi];s|x_0) = v(x_0)/v(z)$. This is a nice results that can be stated more precisely

Proposition 1.1.1. If the process $X(t)$ is a Markov continuous process then the Laplace tranforms $\hat{p}(x,s|x_0,t_0)$ and $\hat{p}_T([-\infty,\xi];s|x_0)$ are given by the products

$$\hat{p}(x,s|x_0,t_0) = \begin{cases} u(x_0)u_1(x) & x > x_0 \\ v(x_0)v_1(x) & x < x_0 \end{cases} \tag{1.55}$$

and

$$\hat{p}_T([-\infty,\xi];s|x_0) = \begin{cases} u(x_0)u(\xi) & x < \xi \\ v(x_0)v(\xi) & x > \xi \end{cases} \tag{1.56}$$

A similar result can be obtained by performing the Laplace transform of eq.s (1.37)

$$\begin{aligned} \hat{p}_T([-\infty,\xi_R];s|x_0) &= \hat{p}_T^{+}([\xi_L,\xi_R];s|x_0) + \hat{p}_T^{-}([\xi_L,\xi_R];s|x_0)\hat{p}_T([-\infty,\xi_R];s|\xi_L) \\ \hat{p}_T([\xi_L,\infty];s|x_0) &= \hat{p}_T^{-}([\xi_L,\xi_R];s|x_0) + \hat{p}_T^{+}([\xi_L,\xi_R];s|x_0)\hat{p}_T([\xi_L,\infty];s|\xi_R) \end{aligned} \tag{1.57}$$

Eqs. (1.57) are 2 linear equations in 2 unknowns. By using the expressions of (1.56) for $\hat{p}_T^{+}([\xi_L,\xi_R];s|x_0)$ and $\hat{p}_T^{-}([\xi_L,\xi_R];s|x_0)$ one gets the results

$$\hat{p}_T^{-}([\xi_L,\xi_R];s|x_0) = \frac{v(\xi_L)u(x_0) - u(\xi_L)v(x_0)}{u(\xi_R)v(\xi_L) - u(\xi_L)v(\xi_R)} \tag{1.58}$$

$$\hat{p}_T^{+}([\xi_L,\xi_R];s|x_0) = \frac{v(x_0)u(\xi_R) - u(x_0)v(\xi_R)}{u(\xi_R)v(\xi_L) - u(\xi_L)v(\xi_R)} \tag{1.59}$$

(1.60)

Moreover, since $\hat{p}_T([\xi_L,\xi_R];s|x_0) = \hat{p}_T^{+}([\xi_L,\xi_R];s|x_0) + \hat{p}_T^{-}([\xi_L,\xi_R];s|x_0)$, we have

$$\hat{p}_T([\xi_L,\xi_R];s|x_0) = \frac{v(x_0)\left(u(\xi_R) - u(\xi_L)\right) - u(x_0)\left(v(\xi_R) - v(\xi_L)\right)}{u(\xi_R)v(\xi_L) - u(\xi_L)v(\xi_R)} \tag{1.61}$$

Symmetrical process

Note that if the process is symmetrical i.e. if $p(x,t|x_0,t_0) = p(-x,t|-x_0,t_0)$, for all x, x_0, t, then $u(x_0) = -v(x_0)$ and if we consider $\xi_L = -\xi_R = -\xi$ the relation above simplifies to

$$\hat{p}_T([-\xi,\xi];s|x_0) = \frac{u(x_0)+u(-x_0)}{u(\xi)+u(-\xi)}. \tag{1.62}$$

At this point we can state the following general result.

Proposition 1.1.2. If the conditional probability $p(x,t|x_0,t_0)$ satisfies the backward Fokker-Planck equation (1.40) with the given boundary conditions, than the functions $u(x_0)$ and $v(x_0)$ can be chosen as any two linearly indipendent solutions of the differential equation

$$\hat{L}^\dagger(x_0)w(x_0) - sw(x_0) = 0 \tag{1.63}$$

1.1.4 Standard procedures to compute the MFPT: a summary

From the previous sections we have seen that the computation of the MFPT can be performed according to (at least) three possible routes:

(i) By computing the distribution function $p(x,t|x_0,t_0)$, then the survival probability $S(t|x_0)$ through the relation

$$S(t|x_0) = \int_\Omega p(x,t|x_0,t_0)dx \tag{1.64}$$

and finally the MFPT through the relation

$$T^{(1)}(x_0) = \int_{\mathbb{R}^+} S(t,|x_0)dt. \tag{1.65}$$

This route is certantly the most complete one since it requires the computation of the full pdf $p(x,t|x_0,t_0)$ first. Given $p(x,t|x_0,t_0)$ the full survival probability is obtained by a simple integration over the whole space and from that all the moments $T^{(m)}(x_0)$ can be computed. The problem of this procedure is that, in general, the computation of $p(x,t|x_0,t_0)$ is not an easy task to perform. We have indeed previously seen that sometimes one has to stop at a complicated expression of the Laplace transform of $p(x,t|x_0,t_0)$ that is difficult to invert.

(ii) By solving the PDE (1.42) with the corresponding boundary conditions for the survival probability $S(t|x_0)$ and then use eq. (1.65) to compute $T^{(1)}(x_0)$. Note that also in this case one can get all the moments $T_n(x_0)$. As in the case of procedure [i], the computation of $S(t|x_0)$ is not, in general an easy task to perform and is some case one has to study the asymtptotic properties of its Laplace transform $S(s|x_0)$.

(iii) By solving the ODE (1.44) for the MFPT. This is in principle the simplest way to compute $T^{(1)}(x_0)$ since it requires to find the solution of an ordinary differential equation. The drawback of this procedure is that only $T^{(1)}(x_0)$ is accessible. For example one cannot get the full survival probability but only its relaxation time approximation $S_{appr}(t|x_0) \simeq e^{-t/T^{(1)}(x_0)}$

In the next examples we will try to compute the MFPT by following all (of some of) the procedure just mentioned.

1.1.5 MFPT for 1d diffusive processes in a finite region

As a first example let us consider the Wiener process defined on the region $x \in [0,L]$ i.e.

$$\Delta x = 2D^{1/2}\Delta W. \tag{1.66}$$

This problem corresponds to a random walk with diffusion constant D. For this process one can find the mean first passage time for the exit through either $x=0$ or $x=L$ from an initial position $x(t_0) = x_0$.

MFPT from route [i]

Following this approach we need the full solution for the probability $p(x,t|x_0,t_0)$ found in section **??** of the previous Chapter:

$$p(x,t|x_0,t_0) = \frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{L}x_0\right)e^{-D\lambda_n^2(t-t_0)}, \tag{1.67}$$

where

$$\lambda_n^2 = \left(\frac{n\pi}{L}\right)^2 \tag{1.68}$$

The survival probability $S(t|x_0)$ can be obtained from the above solution by simply integrating over the whole domain:

$$S(t,x_0) = \int_0^L p(x,t|x_0,t_0)dx \tag{1.69}$$

Note that, since the variables x and t are separated in $p(x,t|x_0,t_0)$, this integration is not going to change the time-dependent factor. Hence the time-dependence of the survival probability must correspond to the one found for $p(x,t|x_0,t_0)$. Since the large-n terms in $p(x,t|x_0,t_0)$ decay more rapidly with time, in the long time limit (i.e. $t >> L^2/D$) only the term with the largest characteristic decay time remains. One can then assume

$$S(t|x_0) \sim e^{-\frac{\pi^2 D(t-t_0)}{L^2}} \sim e^{-t/\tau} \tag{1.70}$$

The characteristic decay time τ of the survival probability in the long time limit is the MFPT of the process since

$$T^{(1)}(x_0) \sim \frac{1}{\tau}\int_{\mathbb{R}^+} te^{-t/\tau}dt = \tau. \tag{1.71}$$

If one is not only interested in the long time limit but in the full expression for $T^{(1)}(x_0)$ it is convenient to insert the full solution in the definition of the first passage time distribution function

$$-dS(t|x_0) = \left(-\int_0^L \partial_t p(x,t|x_0,t_0)dx\right)dt. \tag{1.72}$$

This gives

$$\begin{aligned} -\frac{dS(t|x_0)}{dt} &= \int_0^L \sum_{n=1}^{\infty} D\lambda_n^2 \frac{2}{L}\sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{L}x_0\right)e^{-D\lambda_n^2(t-t_0)}dx \\ &= \sum_{n=1,n,odd}^{\infty} \frac{2D\lambda_n^2}{L}\frac{2L}{n\pi}\sin\left(\frac{n\pi}{L}x_0\right)e^{-D\lambda_n^2(t-t_0)}. \end{aligned} \tag{1.73}$$

The first moment of $-dS(t|x_0)$ gives the MFPT

$$\begin{aligned} T^{(1)}(x_0) = -\int_{t_0}^{\infty} tdS(t|x_0) &= \sum_{n=1,n,odd}^{\infty} \frac{D\lambda_n^2}{L}\frac{4L}{n\pi}\sin\left(\frac{n\pi}{L}x_0\right)\int_{t_0}^{\infty} te^{-D\lambda_n^2(t-t_0)}dt \\ &= \sum_{n=1,n,odd}^{\infty} \frac{4}{D\lambda_n^2 n\pi}\sin\left(\frac{n\pi}{L}x_0\right) \\ &= \sum_{n=1,n,odd}^{\infty} \frac{4L^2}{Dn^3\pi^3}\sin\left(\frac{n\pi}{L}x_0\right). \end{aligned} \tag{1.74}$$

This is a Fourier series that converges to give a value for $T^{(1)}(x_0)$.

A different approach

Suppose the process $X(t)$ is defined over the interval $[-\xi, \xi]$. Since it is a diffusive process the conditional probability satisfies the backward differential equation

$$\partial_t p = \frac{1}{2}\frac{\partial^2 p}{\partial x_0^2} \tag{1.75}$$

By performing a Laplace transform we get eq. (1.63) that in this case becomes

$$\frac{1}{2}\frac{d^2}{dx_0^2}w(x_0) - sw(x_0) = 0. \tag{1.76}$$

Two linearly independent solutions are

$$u(x_0) = e^{-x_0\sqrt{2s}}, \qquad v(x_0) = e^{x_0\sqrt{2s}} = u(-x_0) \tag{1.77}$$

and from eq. (1.62) we get

$$\hat{p}_T([-\xi,\xi]; s|x_0) = \frac{\cosh x_0\sqrt{2s}}{\cosh \xi\sqrt{2s}}, \qquad |x_0| < \xi. \tag{1.78}$$

The inversion of the Laplace transform gives

$$p_T([-\xi,\xi]; t|x_0) = \frac{\pi}{\xi^2}\sum_{j=0}^{\infty}(-1)^j(j+1/2)\cos\left[(j+1/2)\frac{\pi x_0}{\xi}\right]e^{-(j+1/2)^2\pi^2 t/(2\xi^2)} \tag{1.79}$$

By integrating on t we get the probability distribution

$$\begin{aligned}\mathcal{P}([-\xi,\xi]; t|x_0) &= \mathbb{P}\left\{T([-\xi,\xi]|x_0) < t\right\} \\ &= 1 - \frac{2}{\pi}\sum_{j=0}^{\infty}\frac{(-1)^j}{(j+1/2)}\cos\left[(j+1/2)\frac{\pi x_0}{\xi}\right]e^{-(j+1/2)^2\pi^2 t/(2\xi^2)}.\end{aligned} \tag{1.80}$$

This result can be also extended to general $\partial\Omega$ since we can always write $[\xi_L, \xi_R]$ as $[-(\xi_R - \xi_L)/2, (\xi_R - \xi_L)/2]$ giving

$$\mathcal{P}([\xi_L,\xi_R]; t|x_0) = \mathcal{P}\left([-(\xi_R-\xi_L)/2, (\xi_R-\xi_L)/2]; t|x_0 - (\xi_L + \xi + R)/2\right). \tag{1.81}$$

MFPT from route [ii]

In this case the problem consists in solving the PDE

$$\frac{\partial}{\partial t}S(t|x_0) = \hat{L}^\dagger(x_0)S(t|x_0) = D\frac{\partial^2}{\partial x_0^2}S(t|x_0) \tag{1.82}$$

with boundary conditions

$$S(t|0) = S(t|L) = 0. \tag{1.83}$$

and initial condition $S(t_0|x_0) = 1$.

Exercise. Solve equation (1.82) either by using the separation of variables method or the Laplace transform.

MFPT from route [iii] and $S_{app}(t|x_0)$

Following route [iii] we have to solve the ODE for the $T^{(1)}(x_0)$:

$$\hat{L}^{\dagger}_{x_0} T^{(1)}(x_0) = -1 \qquad \leftrightarrow \qquad D\frac{d^2 T^{(1)}(x_0)}{dx_0^2} = -1, \tag{1.84}$$

with boundary conditions $T^{(1)} = 0$ at $x_0 = 0$ and $x_0 = L$. A possible solution is given by the homogeneous solution $Ax_0 + B$ and the non-homogeneous one $-x_0^2/2D$. Hence

$$T^{(1)}(x_0) = -\frac{1}{2D}x_0^2 + Ax_0 + B. \tag{1.85}$$

The boundary conditions give

$$B = 0 \qquad \text{and} \qquad A = \frac{1}{2D}L. \tag{1.86}$$

The MFPT is then

$$T^{(1)}(x_0) = \frac{1}{2D}x_0(L - x_0). \tag{1.87}$$

It is easy to see that (1.74) is the Fourier series of this function. Note that if $L = \infty$ the MFPT is infinite. Given $T^{(1)}(x_0)$ one can approximate the survival probability $S(t|x_0)$ as

$$S_{app}(t|x_0) \sim \exp\left(-t/T^{(1)}(x_0)\right). \tag{1.88}$$

1.1.6 Escape from a symmetric barrier: Kramer's formula

Consider a Brownian particle in symmetric potential $U(x) = U(-x)$. This will give rise to a drift velocity $v(x) = -\mu\frac{dU}{dx}$ where $\mu = D/k_B T$ is the mobility and D the diffusion constant. Suppose the potential has a minimum $U = 0$ at $x = 0$ with $U''(0) > 0$ and a two equal maxima $U = E > 0$ at $x = \pm x_M$ with $U''(x_M) < 0$. If the particle starts at the origin compute the mean first passage time $T^{(1)}(0)$ to reach one of the barriers at $x = \pm x_M$ (and the escape from the well with probability 1/2). In particular We first derive the general formula

$$\boxed{T^{(1)}(0) = \frac{1}{D}\int_0^{x_M} dx e^{U(x)/k_B T} \int_0^{x} dy e^{-U(y)/k_B T}} \tag{1.89}$$

In the over-damped limit the Fokker-Planck equation for a Brownian particle in an external field $F(x) = -U'(x)$ is given by the Smoluchowsky equation (**??**)

$$\frac{\partial}{\partial t}p(x,t|0,0) = \frac{D}{k_B T}\frac{\partial}{\partial x}\left(U'(x)p(x,t|0,0)\right) + D\frac{\partial^2}{\partial x^2}p(x,t|0,0) \tag{1.90}$$

where in (**??**) we have made the following changes: $U'(x) = F(x)$, $D = \frac{\sigma^2}{2\gamma^2 m^2}$ and $\frac{1}{\gamma m} = \frac{D}{k_B T}$. Looking for the fundamental solution we consider the initial condition $p(x,0) = \delta(x)$. Moreover the BC are absorbing at the exit points, i.e. $p(\pm x_M, t|0,0) = 0$. Following eq. (**??**) We can write the Smoluchowskii equation in the form

$$\frac{\partial}{\partial t}p(x,t|0,0) = \hat{L}_{FP}(x)p(x,t|0,0) \tag{1.91}$$

where

$$\hat{L}_{FP}(x) = D\frac{\partial}{\partial x}\left[e^{-U(x)/k_B T}\frac{\partial}{\partial x}\left(e^{U(x)/k_B T}\right)\right]. \tag{1.92}$$

By applying the operator $\hat{L}_{FP}(x)$ on both sides of the relation for $g_0(x|x_0)$ we get

$$\hat{L}_{FP}(x)g_0(x|0) = \int_0^{\infty} \hat{L}_{FP}(x)p(x,t|0,0)dt = \int_0^{\infty}\frac{\partial p}{\partial t}dt = -p(x,0|0,0) = -\delta(x). \tag{1.93}$$

Using expression (1.92) for $\hat{L}_{FP}$ it is easy to solve for $g_0(x,0)$ giving

$$g_0(x|0) = \frac{e^{-U(x)/k_BT}}{D}\int_{-x_M}^{x_M} e^{U(y)/k_BT}\left[\int_0^y \delta(z)dz\right]dy \tag{1.94}$$

The MFPT (or escape time) is then given by

$$\begin{aligned} T^{(1)}(0) &= \int_{-x_M}^{x_M} g_0(x|0)dx = 2\int_0^{x_M} g_0(x|0)dx \\ &= \frac{1}{D}\int_0^{x_M} e^{-U(x)/k_BT}\left[\int_{-x_M}^{x_M} e^{U(y)/k_BT}dy\right]dx \end{aligned} \tag{1.95}$$

By performing a partial integration and remembering that $U(0)=0$, $U'(0)=0$ we get

$$\begin{aligned} T^{(1)}(0) &= \frac{1}{D}\left[\left(\int_0^x e^{-U(y)/k_BT}dx\right)\times\left(\int_x^{x_M} e^{U(y)/k_BT}dy\right)\right]_0^{x_M} \\ &+ \frac{1}{D}\int_0^{x_M} e^{U(x)/k_BT}\left[\int_0^x e^{-U(y)/k_BT}dy\right]dx \end{aligned} \tag{1.96}$$

Hence

$$\boxed{T^{(1)}(0) = \frac{1}{D}\int_0^{x_M} dx e^{U(x)/k_BT}\int_0^x dy e^{-U(y)/k_BT}} \tag{1.97}$$

Let us now consider the low k_BT limit. As $k_BT \to 0$ the integrals in the formula are dominated by the extreme values of the exponents. We can then use the saddle point approximation to the evaluate the integrals as follows:

$$\int_0^x e^{-U(y)/k_BT}dy \sim \frac{1}{2}\sqrt{\frac{2\pi k_BT}{U''(0)}}e^{-U(0)/k_BT} = \sqrt{\frac{\pi k_BT}{2U''(0)}} \tag{1.98}$$

Hence

$$\begin{aligned} \int_0^{x_M} dx e^{U(x)/k_BT}\int_0^x dy e^{-U(y)/k_Bt} &\sim \sqrt{\frac{\pi k_BT}{2U''(0)}}\int_0^{x_M} e^{U(x)/k_BT}dx \\ &\sim \sqrt{\frac{\pi k_BT}{2U''(0)}}\frac{1}{2}\sqrt{-\frac{2\pi k_BT}{U''(x_M)}}e^{U(x_M)/k_BT}. \end{aligned} \tag{1.99}$$

Finally, the mean-first passage time in the limit $k_BT \to 0$, is, at zero order:

$$\boxed{T^{(1)}(0) = \frac{\pi k_BT}{2D\sqrt{U''(0)U''(x_M)}}e^{U(x_M)/k_BT} \propto e^{U(x_M)/k_BT}} \tag{1.100}$$

In general

$$\boxed{T^{(1)}(0) = \frac{\pi k_BT}{2D\sqrt{U''(x_{xmain})|U''(x_{max})|}}e^{\Delta U/k_BT}} \tag{1.101}$$

where $\Delta T = U(x_{max} - U(x_{min})$. Equation above is known as **Kramer's formula.** Sometimes it is written in terms of the **escape rate R**:

$$\boxed{R = 1/T^{(1)}(0) = \frac{2D\sqrt{U''(x_{min})|U''(x_{max})|}}{\pi k_BT}e^{-\Delta U/k_BT}}. \tag{1.102}$$

It is possible to improve the saddle point approximation and computing the first correction to the leading term. This can be done imply to keeping one term in the expansion of the exponential. In order to do this let us consider the relation

$$\begin{aligned}\int_{\mathbb{R}} e^{-ax^2+bx^3+cx^4}dx &\sim \int_{\mathbb{R}}\left(1+bx^3+cx^4+\frac{b^2x^6}{2}\right)e^{-ax^2}dx \\ &= \sqrt{\frac{\pi}{a}}\left(1+\frac{3c}{4a^2}+\frac{15b^2}{16a^3}\right). \end{aligned} \tag{1.103}$$

We now use again the saddle point approximation with the above formula

$$\int_0^x e^{-U(y)/k_BT}dy \sim \frac{1}{2}\sqrt{2\pi k_BT}U''(0)\left(1-\frac{k_BTU^{(IV)}(0)}{8(U''(0))^2}+\frac{5k_BT(U^{III}(0))^2}{(U''(0)^3)}\right)e^{-U(0)/k_BT} \tag{1.104}$$

On the other hand the well is symmetric and $U^{III}(0) =$ giving

$$\int_0^x e^{-U(y)/k_BT}dy \sim \sqrt{\frac{\pi k_BT}{2U''(0)}}\left(1-\frac{k_BTU^{(IV)}(0)}{8(U''(0))^2}\right) \tag{1.105}$$

Similarly

$$\begin{aligned}\int_0^{x_M} e^{U(x)/k_BT}dx &\sim \frac{1}{2}\sqrt{-2\pi k_BT}U''(x_M)\left(1+\frac{k_BTU^{(IV)}(x_M)}{8(U''(x_M))^2}-\frac{5k_BT(U^{III}(x_M))^2}{(U''(x_M)^3)}\right)e^{U(x_M)/k_BT} \\ &\sim \sqrt{\frac{\pi k_BT}{2U''(x_M)}}\left(1+\frac{k_BTU^{(IV)}(x_M)}{8(U''(x_M))^2}-\frac{5k_BT(U^{(III)}(x_M))^2}{24(U''(x_M))^3}\right)\end{aligned} \tag{1.106}$$

We finally have

$$\begin{aligned}T^{(1)}(0) &\sim \frac{1}{R_0(T)}\left(1-\frac{k_BTU^{(IV)}(0)}{8U''(0)^2}\right)\left(1+\frac{k_BTU^{(IV)}(x_M)}{U''(x_M)^2}-\frac{5k_BTU^{(III)}(x_M)^2}{24U''(x_M)^3}\right) \\ &\sim \frac{1}{R_0(T)}\left[1+\frac{k_BT}{8}\left(\frac{U^{(IV)}(x_M)}{(U''(x_M)^2)}-\frac{U^{(IV)}(0)}{(U''(0))^2}-\frac{5(U^{(III)}(x_M))^2}{3(U''(x_M))^3}\right)\right]\end{aligned} \tag{1.107}$$

Hence

$$\boxed{R(T) \sim R_0(T)\left[1-\frac{k_BT}{8}\left(\frac{U^{(IV)}(x_M)}{(U''(x_M)^2)}-\frac{U^{(IV)}(0)}{(U''(0))^2}-\frac{5(U^{(III)}(x_M))^2}{3(U''(x_M))^3}\right)\right]} \tag{1.108}$$

1.2 First passage problem for a 1d overdamped motion with external (periodic) potential

Let us now consider the 1D overdamped Brownian motion for a particle subject to an external potential $V(x)$ than later we will specify to be periodic or tilted periodic. The Smoluchowski equation is

$$\partial_t p(x,t|x_0,t_0) = \hat{L}_{FP}(x)p(x,t|x_0,t_0) \tag{1.109}$$

with

$$\hat{L}_{FP}(x) = \frac{\partial}{\partial x}\left\{D(x)e^{-\beta V(x)}\frac{\partial}{\partial x}e^{\beta V(x)}\right\}. \tag{1.110}$$

Note that, in order to keep the problem as much general as possible, we consider the diffusion coefficient to be a function of x. According to our previous results the adjiont operator is

$$\hat{L}^{\dagger}(x) = e^{\beta V(x)}\frac{\partial}{\partial x}\left\{\frac{\partial}{\partial x}e^{-\beta V(x)}\right\}. \tag{1.111}$$

and the differential equation for the mean first passage time for a process starting at x_0 is

$$\hat{L}^\dagger(x)T^{(1)}(x_0) = -1 \tag{1.112}$$

i.e.

$$\frac{\partial}{\partial x_0}\left\{D(x_0)e^{-\beta V(x_0)}\frac{\partial}{\partial x_0}\right\}T^{(1)}(x_0) = -e^{-\beta V(x_0)}. \tag{1.113}$$

By integrating on both side

$$D(x_0)e^{-\beta V(x_0)}\frac{\partial}{\partial x_0}T^{(1)}(x_0) = -\int_a^{x_0} e^{-\beta V(z)}dz + C_1 \tag{1.114}$$

where a is an arbitrary point in the domain $[\xi_L, \xi_R]$. In the specific we will consider the motion in the region $\Omega = [-\infty, \infty]$ where we have reflecting boundary consitions at the extremities. On the other hand, if we want to look at the mean first passage problem for the particle to reach the point $x = b$ starting from an initial point $x_0 < b$, it is convenient to restrict the motion to the subregion $[-\infty, b]$ where $x = -\infty$ is reflecting and $x = b$ is absorbing. In this case the constant C_1 is determined by imposing that the boundary at $x = -\infty$ is reflecting: $dT^{(1)}(x_0)/dx_0|_{x_0\to-\infty} = 0$. Hence

$$C_1 = \int_a^{-\infty} e^{-\beta V(z)}dz \tag{1.115}$$

and by plugging back

$$\frac{\partial}{\partial x_0}T^{(1)}(x_0) = \frac{e^{\beta V(x_0)}}{D(x_0)}\left\{-\int_a^{x_0} e^{-\beta V(z)}dz + \int_a^{-\infty} e^{-\beta V(z)}dz\right\} \tag{1.116}$$

i.e.

$$\frac{\partial}{\partial x_0}T^{(1)}(x_0) = -\frac{e^{\beta V(x_0)}}{D(x_0)}\int_{-\infty}^{x_0} e^{-\beta V(z)}dz. \tag{1.117}$$

By integrating again on both sides

$$T^{(1)}(x_0) = -\int_a^{x_0}\frac{e^{\beta V(y)}}{D(y)}dy\int_{-\infty}^{y} e^{-\beta V(z)}dz + C_2. \tag{1.118}$$

If we look at the mean first passage time for the system to reach point b, starting from the initial condition x_0 an obvious condition is $T^{(1)}(x_0 = b) = 0$ i.e.

$$-\int_a^{b}\frac{e^{\beta V(y)}}{D(y)}dy\int_{-\infty}^{y} e^{-\beta V(z)}dz + C_2 = 0 \tag{1.119}$$

$$C_2 = \int_a^{b}\frac{e^{\beta V(y)}}{D(y)}dy\int_{-\infty}^{y} e^{-\beta V(z)}dz \tag{1.120}$$

Finally

$$T^{(1)}(x_0 \to b) = \int_{x_0}^{b}\frac{e^{\beta V(y)}}{D(y)}dy\int_{-\infty}^{y} e^{-\beta V(z)}dz. \tag{1.121}$$

Moreover, from the general recursive relation,

$$\hat{L}^\dagger_{FP}(x_0)T^{(m)}(x_0) = -mT^{(m-1)}(x_0) \tag{1.122}$$

one obtains

$$T^{(m)}(x_0 \to b) = m\int_{x_0}^{b}\frac{e^{\beta V(y)}}{D(y)}dy\int_{-\infty}^{y} e^{-\beta V(z)}T^{(m)}(z \to b)dz. \tag{1.123}$$

with $T^{(0)}(y \to b) = 1$.

1.2.1 Periodic potential

Suppose $V(x)$ is periodic: $V(x+L) = V(x)$ or tilted periodic $V(x+L) = V(x) + FL$. In this case some semplification are possible for the integral

$$I(y) \equiv \frac{e^{\beta V(y)}}{D(y)} \int_{-\infty}^{y} e^{-\beta V(z)} dz. \tag{1.124}$$

TODO

1.3 First passage problem for Ornstein-Uhlenbeck processes

Let us consider the most general O-U process defined by the following SDE

$$dY(t) = (-\gamma Y(t) + \mu)dt + \sigma dW \tag{1.125}$$

where dW is the increment of the usual Wiener process. To remove the constant μ from the process it is sufficient to consider the stochastic process $X(t)$ defined as

$$X(t) = Y(t) - \mu/\gamma \tag{1.126}$$

giving

$$dX(t) = -\gamma X(t)dt + \sigma dW \tag{1.127}$$

The corresponding Fokker-Planck equation is

$$\frac{\partial}{\partial t} p(x,t|x_0,t_0) = \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2} p(x,t|x_0,t_0) - \frac{\partial}{\partial x} \left[(\mu - \gamma x) p(x,t|x_0,t_0)\right] \tag{1.128}$$

and with the initial condition $\lim_{t\to t_0} p(x,t|x_0,t_0) = \delta(x - x_0)$ and the natural BC gives the solution

$$p(x,t|x_0,t_0) = \left[\pi \frac{\sigma^2}{\gamma}\left(1 - e^{-2\gamma t}\right)\right]^{-1/2} \exp\left[-\frac{\left[x - \mu/\gamma + (\mu/\gamma - x_0)e^{-\gamma t}\right]^2}{\frac{\sigma^2}{\gamma}\left(1 - e^{-2\gamma t}\right)}\right] \tag{1.129}$$

In other words $p(x,t|x_0,t_0) \in \mathbb{N}\left(\mathbb{E}(X), Var(X)\right)$ with

$$\mathbb{E}(X(t)|X(0) = x_0) = \frac{\mu}{\gamma} - \left(\frac{\mu}{\gamma} - x_0\right) e^{-\gamma t} \tag{1.130}$$

and

$$Var(X) = \frac{\sigma^2}{2\gamma}\left(1 - e^{-2\gamma t}\right). \tag{1.131}$$

Moreover

$$\begin{aligned} \mathbb{E}\left\{X(t)X(\tau)\right\} &= \frac{\mu^2}{\gamma^2} + \frac{\mu}{\gamma}\left(x_0 - \frac{\mu}{\gamma}\right)\left(e^{-\gamma t} + e^{-\gamma \tau}\right) \\ &+ \left[\left(x_0 - \frac{\mu}{\gamma}\right)^2 - \frac{\sigma^2}{2\gamma}\right] e^{-\gamma(t+\tau)} + \frac{\sigma^2}{2\gamma} e^{-\gamma|t-\tau|} \end{aligned} \tag{1.132}$$

One can immediatly see that the O-U process admits a steady state ($\gamma t >> 1$) solution.

In order to solve the problem for the first passage time of the O-U process we consider the Laplace transform of the pdf $p_T(\partial\Omega, t|x_0)$

$$\hat{p}_T(\partial\Omega, s|x_0) = \int_{\mathbb{R}^+} p_T(\partial\Omega, t|x_0) e^{-st} dt. \tag{1.133}$$

We have seen previously that $\hat{p}_T(\partial\Omega, s|x_0)$ satisfies eq. (1.49) where in this case

$$\hat{L}^{\dagger}_{FP}(x) = D^{(1)}(x)\frac{\partial}{\partial x} + D^{(2)}(x)\frac{\partial^2}{\partial x^2} = (-\mu + \gamma x_0)\frac{d}{dx_0} + \frac{\sigma^2}{2}\frac{d^2}{dx_0^2}. \tag{1.134}$$

Hence the equation to be solved in the Laplace space is

$$\frac{\sigma^2}{2}\frac{d^2}{dx_0^2}\hat{p}_T(\partial\Omega, s|x_0) + (-\mu + \gamma x_0)\frac{d}{dx_0}\hat{p}_T(\partial\Omega, s|x_0) - s\hat{p}_T(\partial\Omega, s|x_0) = 0. \tag{1.135}$$

The BC conditions to be imposed on this equation depend on the first passage time problem considered: If for example $\partial\Omega = [r, \xi_R]$ with r reflecting and ξ_R absorbing the corresponding BC are

$$\lim_{x_0\to\xi_R} \hat{p}_T([r, \xi_R], s|x_0) = 1, \qquad \lim_{x_0\to r} \hat{p}_T([r, \xi_R], s|x_0) = 0. \tag{1.136}$$

If, on the other hand, two absorbing BC are considered (i.e. $\partial\Omega = [\xi_L, \xi_R]$) the BC become

$$\lim_{x_0\to\xi_R} \hat{p}_T([r, \xi_R], s|x_0) = 1, \qquad \lim_{x_0\to\xi_L} \hat{p}_T([r, \xi_R], s|x_0) = 1. \tag{1.137}$$

To solve the above equation we first consider the following change of variables

$$y_0 = x_0 - \mu/\gamma \tag{1.138}$$

This gives

$$\frac{\sigma^2}{2}\frac{d^2}{dy_0^2}\hat{p}_T(\partial\Omega, s|y_0) + \gamma y_0\frac{d}{dy_0}\hat{p}_T(\partial\Omega, s|y_0) - s\hat{p}_T(\partial\Omega, s|y_0) = 0. \tag{1.139}$$

Clearly $\lim_{x_0\to a}$ is replaced by $\lim_{y_0\to a-\mu/\gamma}$. Following a typical procedure used to solve the parabolic cylinder equation we perform the change of variable

$$y_0 = -\left(\sigma^2 w_0/\gamma\right)^{1/2} \tag{1.140}$$

that inserting in (1.139) gives

$$w_0\frac{d^2}{dw_0^2}\hat{p}_T(\partial\Omega, s|w_0) + (1/2 - w_0)\frac{d}{dw_0}\hat{p}_T(\partial\Omega, s|w_0) - \frac{s}{\gamma}\hat{p}_T(\partial\Omega, s|w_0) = 0. \tag{1.141}$$

If we perform a further set of transformation

$$\hat{p}_T(\partial\Omega, s|w_0) = e^{w_0/2}\hat{u}(\partial\Omega, s|w_0) \tag{1.142}$$

$$w_0 = z_0^2/2, \tag{1.143}$$

we finally get

$$\frac{d^2}{dz_0^2}\hat{u}(\partial\Omega, s|z_0) + \left(-s/\gamma + 1/2 - z_0^2/4\right)\hat{u}(\partial\Omega, s|z_0) = 0. \tag{1.144}$$

This last equation is the so called *Weber equation* and its general solution is a linear combination of the two independent soution $D_{-s/\gamma}(z_0)$ and $D_{-s/\gamma}(-z_0)$ where $D_\eta(x)$ is the *Parabolic Cylinder Function* (or Weber function) (see Appendix) Hence

$$\hat{u}(\partial\Omega; s|z_0) = AD_{-s/\gamma}(z_0) + BD_{-s/\gamma}(-z_0). \tag{1.145}$$

In order to get the coefficients A and B we should look at the BC considered.

Case I $\partial\Omega = [r, \xi]$.

In this case we should impose the BC

$$\lim_{z_0\to z_\xi} \hat{u}([r, \xi]; s|z_0)e^{z_0^2/4} = 1,$$

$$\lim_{z_0\to z_r} \hat{u}([r, \xi]; s|z_0)e^{z_0^2/4} = 0. \tag{1.146}$$

This gives

$$\begin{aligned} AD_{-s/\gamma}(z_\xi) + BD_{-s/\gamma}(-z_\xi) &= e^{-z_\xi^2/4} \\ AD_{-s/\gamma}(z_r) + BD_{-s/\gamma}(-z_r) &= 0. \end{aligned} \tag{1.147}$$

Solving with respect to A and B we have:

$$\begin{aligned} A &= e^{-z_\xi^2/4} \frac{D(-z_r)}{D(z_\xi)D(-z_r) - D(z_r)D(-z_\xi)} \\ B &= -e^{-z_\xi^2/4} \frac{D(z_r)}{D(z_\xi)D(-z_r) - D(z_r)D(-z_\xi)} \end{aligned} \tag{1.148}$$

where we have omitted the subscripts $-s/\gamma$ for simplicity. By plugging back in the solution for $\hat{u}(\partial\Omega; s|z_0)$ we should get

$$\hat{u}(\partial\Omega; s|z_0) = e^{-z_\xi^2/4} \left[\frac{D(z_0)D(-z_r) - D(z_r)D(-z_0)}{D(z_\xi)D(-z_r) - D(z_r)D(-z_\xi)} \right]. \tag{1.149}$$

The expression above is quite complicated but in the limit $z_r \to -\infty$ it can be simplified a lot. Indeed it is known that the asymptotic expansion of the Weber functions are

$$\begin{aligned} D_{-s/\gamma}(x) &= e^{-x^2/4} x^{-s/\gamma} \left[1 + O\frac{1}{x^2} \right] \\ D_{-s/\gamma}(-x) &= \frac{\sqrt{2\pi}}{\Gamma(s/\gamma)} e^{-x^2/4} x^{s/\gamma+1} \left[1 + O\frac{1}{x^2} \right] \end{aligned} \tag{1.150}$$

Hence

$$\frac{D_{-s/\gamma}(x)}{D_{-s/\gamma}(-x)} = x \left(1 + O\frac{1}{x^2} \right). \tag{1.151}$$

Suppose we consider the case $r \to -\infty$ and take $b = -z_r$. From the expression of A and B we finally get

$$\begin{aligned} A &= e^{-z_\xi^2/4} \frac{1}{D(z_\xi) - \frac{D(z_r)}{D(-z_r)} D(-z_\xi)} \to e^{-z_\xi^2/4} \frac{1}{D(z_\xi)} \\ B &= e^{-z_\xi^2/4} \frac{1}{D(z_\xi)\frac{D(-z_r)}{D(z_r)} - D(-z_\xi)} \to 0 \end{aligned} \tag{1.152}$$

The solution for $\partial\Omega = [-\infty, \xi]$ is then

$$\hat{u}(\partial\Omega; s|z_0) = e^{-z_\xi^2/4} \frac{D(-z_0)}{D(-z_\xi)}. \tag{1.153}$$

and since $\hat{p}_T(\partial\Omega; s|z_0) = e^{z_0^2/2} \hat{u}(\partial\Omega; s|z_0)$ we have

$$\hat{p}_T(\partial\Omega; s|z_0) = \exp\left(\frac{z_0^2 - z_\xi^2}{4} \right) \frac{D(-z_0)}{D(-z_\xi)}. \tag{1.154}$$

Note that in the case we consider $\partial\Omega = [\xi, +\infty]$ (i.e. $xz_0 > z_\xi$), the solution would be

$$\hat{p}_T(\partial\Omega; s|z_0) = \exp\left(\frac{z_0^2 - z_\xi^2}{4} \right) \frac{D(z_0)}{D(z_\xi)}. \tag{1.155}$$

Going backwards in the sequence of transformations i.e.

$$z = -2^{1/2}\frac{y\gamma^{1/2}}{\sigma} = -\frac{(2\gamma)^{1/2}}{\sigma}(x_0 - \mu/\gamma) \tag{1.156}$$

we finally get

$$\hat{p}_T(\partial\Omega; s|x_0) = \exp\left[\frac{\gamma}{2\sigma^2}\left((x_0-\mu/\gamma)^2 - (\xi-\mu/\gamma)^2\right)\right]\frac{D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}(x_0-\mu/\gamma)\right]}{D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}(\xi-\mu/\gamma)\right]} \tag{1.157}$$

Case II $\partial\Omega = [\xi_L, \xi_R]$ In this case we should impose the BC

$$\begin{aligned} \lim_{z_0\to z_{\xi_L}} \hat{u}([\xi_L,\xi_R]; s|z_0)e^{z_0^2/4} &= 1, \\ \lim_{z_0\to z_{\xi_R}} \hat{u}([\xi_L,\xi_R]; s|z_0)e^{z_0^2/4} &= 1. \end{aligned} \tag{1.158}$$

This gives

$$\begin{aligned} AD_{-s/\gamma}(z_{\xi_L}) + BD_{-s/\gamma}(-z_{\xi_L}) &= e^{-z_{\xi_L}^2/4} \\ AD_{-s/\gamma}(z_{\xi_R}) + BD_{-s/\gamma}(-z_{\xi_R}) &= e^{-z_{\xi_R}^2/4}. \end{aligned} \tag{1.159}$$

and by solving with respect to A and B gives

$$\begin{aligned} A &= -\frac{D(-z_L)e^{-z_R^2/4} - D(-z_R)e^{-z_L^2/4}}{D(z_L)D(-z_R) - D(z_R)D(-z_L)} \\ B &= \frac{D(z_L)e^{-z_R^2/4} - D(z_R)e^{-z_L^2/4}}{D(z_L)D(-z_R) - D(z_R)D(-z_L)} \end{aligned}$$

By plugging back these expressions in the solution for $\hat{u}(\partial\Omega; s|z_0)$ we obtain

$$\hat{u}([\xi_L,\xi_R]; s|z_0) = \frac{\left[\left(D(z_L)e^{-z_R^2/4} - D(z_R)e^{-z_L^2/4}\right)D(-z_0) - \left(D(-z_L)e^{-z_R^2/4} - D(-z_R)e^{-z_L^2/4}\right)D(z_0)\right]}{D(z_L)D(-z_R) - D(z_R)D(-z_L)} \tag{1.160}$$

Note that in the more symmetric situation $\partial\Omega = [-\xi, \xi]$ by changing $z_R = z_\xi$, $z_L = -z_\xi$ in the above equation and symplifying we get

$$\hat{u}([-z_\xi, z_\xi]; s|z_0) = e^{-z_\xi^2/4}\frac{D(-z_0) + D(z_0)}{D(-z_\xi) + D(z_\xi)} \tag{1.161}$$

Note. We could have reached the same results by referring to equation (1.62) where $u(z)$ replaced by $D(z)$.

Going backwards along the sequence of tranformations we obtain

$$\hat{p}([-\xi,\xi]; s|x_0) = e^{\left[\frac{\gamma}{2\sigma^2}\left((x_0-\mu/\gamma)^2-(\xi-\mu/\gamma)^2\right)\right]}\frac{D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}(x_0-\mu/\gamma)\right] + D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}(\mu/\gamma - x_0)\right]}{D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}(\xi-\mu/\gamma)\right] + D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}(\mu/\gamma - \xi)\right]}. \tag{1.162}$$

The above solution seems very difficult to be inverted. To simplify the situation let us suppose $\mu = 0$ and $x_0 = 0$. Then

$$\hat{p}([-\xi,\xi]; s|0) = \frac{D_{-s/\gamma}(0) + D_{-s/\gamma}[0]}{D_{-s/\gamma}\left[\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}\xi\right] + D_{-s/\gamma}\left[-\left(\frac{2\gamma}{\sigma^2}\right)^{1/2}\xi\right]}. \tag{1.163}$$

If we call $a_\xi = \left(\frac{2\gamma}{\sigma^2}\right)^{1/2} \xi$ we have to calculate the inverse transform of the function

$$\hat{p}([-\xi, \xi]; s|0) = \frac{2D_{-s/\gamma}(0)}{D_{-s/\gamma}(a_\xi) + D_{-s/\gamma}(-a_\xi)}. \tag{1.164}$$

Exercises

1. Consider the $d = 1$ stochastic process $X(t)$ that evolves within the domain $[a, b]$ according to the Langevin equation

$$\Delta x(t) = F(x) + \Delta W \tag{1.165}$$

where

$$F(x) = -\left(\frac{dU(x)}{dx}\right) \tag{1.166}$$

is a force due to the potential $U(x)$ and the corresponding FP equation is

$$\frac{\partial}{\partial t}p(x,t|x_0,t_0) = -\left(\frac{\partial}{\partial x}\left(F(x)p(x,t|x_0,t_0)\right)\right) + \frac{D}{2}\left(\frac{\partial^2}{\partial x^2}p(x,t|x_0,t_0)\right) \tag{1.167}$$

where D is the 1d diffusion coefficient. Compute the mean first passage time of the process by using the adjoint operator and solve the equation

$$\hat{L}_F^{dagger} P(x_0) T^{(1)}(x_0) = -1 \tag{1.168}$$

for the three cases

- a reflecting and b absorbing
- a absorbing and b reflecting
- a and b both absorbing

As an application consider the cases in which $U = -x$ and $U = -\frac{1}{2}x^2$

2. Find the mean of the minimum first passage time for a system of N random walks all starting at x_0 and living in the region $x \in [0, L]$.

Solution. From the definition of the first passage time, the minimum first passage time is the time when the first among the N walkers reaches the boundaries i.e.

$$\tau_{min} = \min\{T^{(1)}, \cdots, T^{(N)}\} \tag{1.169}$$

where $T^{(i)}$ is the first passage time of the i-esim walker. τ_{min} is clearly related to the probability $S_N(t|x_0)$ that N walkers, all starting at x_0 survive at time t. If the N walkers are independent this probability is simply given by the product of the individual survival probabilities $S(t|x_0)$ previously computed, i.e.

$$S_N(t|x_0) = S(t|x_0)^N. \tag{1.170}$$

Therefore, the PDF of the minimum first passage time is

$$f_N(t|x_0) = -\frac{d}{dt}S(t|x_0)^N = Nf(t|x_0)S(t|x_0)^{N-1} \tag{1.171}$$

The mean of the minimum first passage time is then

$$\langle\tau(x_0)\rangle = \int_0^\infty tf_N(t|x_0)dt = N\int_0^\infty f(t|x_0)S(t|x_0)^{N-1}dt \tag{1.172}$$

Chapter 2

First passage problems in $d > 1$

Let us consider now the first passage problem for stochastic processes defined on $\mathbb{R}^d$. In this case we suppose that the stochastic process is defined on a region $\Omega \subset \mathbb{R}^d$ with boundary $\partial\Omega$. The boundary can be sufficiently complex and in general can be the union of different subsets $\partial\Omega = \bigcup \Gamma_i$. To fix the idea consider a stochastic process $\vec{X}(t)$ defined on a subregion of $\mathbb{R}^3$ delimitated by two spherical surfaces Γ_{ext} and Γ_{in}. In this case $\partial\Omega = \Gamma_{ext} \bigcup \Gamma_{in}$ with $\Gamma_{ext} \bigcap \Gamma_{in} = \emptyset$. The definitions are similar to the ones presented for the $d = 1$ case the only difference being in the determination of the BC.

Definition. The first passage time of a stochastic process $\vec{X}(t)$ defined on a domain Ω of boundary $\partial\Omega$ and whose starting point is $\vec{X}(0) = \vec{x}_0$ is the time at which the stochastic variable $\vec{X}(t)$ first leaves a specific domain Ω through its boundary $\partial\Omega$.

Following the $d = 1$ we can consider some particular boundaries $\partial\Omega$ and define $T(\partial\Omega, \vec{x_0})$ accordingly.

- Suppose $\partial\Omega = \Gamma_{ext} \bigcup \Gamma_{in}$ where Γ_{ext} is a reflecting boundary (that can go also to infinity). If one is interested in looking at the stochastic process reaching for the first time the boundary Γ_{in}, the first passage time can be defined as

$$T(\Gamma_{in}, \vec{x_0}) = \sup \left\{ t \geq 0 | \vec{X}(\tau) \in \Omega / \Gamma_{in} \right\} \tag{2.1}$$

  or

$$T(\Gamma_{in}, \vec{x_0}) = \inf \left\{ t \geq 0 | \vec{X}(t) \in \Gamma_{in} \right\} \tag{2.2}$$

- Another case is when both boundaries are absorbing. In analogy with the second case described in the previous chapter we then define

$$T(\Gamma_{in}, \Gamma_{ext}, \vec{x_0}) = \sup \left\{ t \geq 0 | \vec{X}(\tau) \in Int(\Omega) \right\} \tag{2.3}$$

  or

$$T(\Gamma_{in}, \Gamma_{ext}, \vec{x_0}) = \inf \left\{ t \geq 0 | \vec{X}(t) \in \Gamma_{in} \text{ or } \vec{X}(t) \in \Gamma_{ext} \right\} \tag{2.4}$$

The definition of the probability distribution for $T(\partial\Omega, \vec{x_0})$ is similar to the one defined for $d = 1$.

Probabiity distribution of $T(\partial\Omega, \vec{x}_0)$

The probability distribution of the random variable $T(\partial\Omega, \vec{x}_0)$ is defined as

$$\mathcal{T}(\partial\Omega, t | \vec{x}_0) = \mathbb{P} \left\{ T(\partial\Omega, \vec{x}_0) < t | \vec{X}(0) = \vec{x}_0 \right\} \tag{2.5}$$

and its PDF

$$p_T(\partial\Omega, t|\vec{x}_0)dt = \mathbb{P}\left\{t \geq T(\partial\Omega, \vec{x}_0) \geq t + dt|\vec{X}(0) = \vec{x}_0\right\} \equiv d\mathcal{T}(\partial\Omega, t|x_0) \tag{2.6}$$

Note. The density distribution $p_T(\partial\Omega, t|\vec{x}_0)$ is known, in diffusion controlled reaction problems, as the *reaction rate* of the process.

Survival probability

As in $d = 1$ the **survival probability** of $\vec{X}(t)$ started at $\vec{x}_0$ and with boundary $\partial\Omega$ is given by

$$S(\partial\Omega, t|x_0) \equiv 1 - \mathcal{T}(\partial\Omega, t|x_0) = \mathbb{P}\left\{T(\partial\Omega, \vec{x}_0) > t|\vec{X}(0) = \vec{x}_0\right\} \tag{2.7}$$

Clearly

$$p_T(\partial\Omega, t|\vec{x}_0)dt = d\left(1 - S(\partial\Omega, t|\vec{x}_0)\right) - -dS(\partial\Omega, t|\vec{x}_0) \tag{2.8}$$

Hence

$$\boxed{p_T(\partial\Omega, t|\vec{x}_0)dt = -\frac{\partial}{\partial t}S(\partial\Omega, t|x_0)dt.} \tag{2.9}$$

Moments of the distribution $\mathcal{T}(\partial\Omega, t|x_0)$

The first moment or **mean first passage time** (MFPT) is here defined as

$$\mathbb{E}\left\{T(\partial\Omega, \vec{x}_0)\right\} \equiv T^{(1)}(\partial\Omega, \vec{x}_0) = \int_0^\infty t p_T(\partial\Omega, t|\vec{x}_0)dt = -\int_0^\infty t\frac{\partial}{\partial t}S(\partial\Omega, t|\vec{x}_0)dt. \tag{2.10}$$

Similarly,

$$\mathbb{E}\left\{T(\partial\Omega, \vec{x}_0)^m\right\} \equiv T^{(m)}(\partial\Omega, \vec{x}_0) = \int_0^\infty t^m p_T(\partial\Omega, t|\vec{x}_0)dt = -\int_0^\infty t^m\frac{\partial}{\partial t}S(\partial\Omega, t|\vec{x}_0)dt. \tag{2.11}$$

If we integrate the last equation by parts we get

$$T^{(m)}(\partial\Omega, \vec{x}_0) = t^m S(\partial\Omega, t|\vec{x}_0)\,|_0^\infty + \int_0^\infty t^{m-1}S(\partial\Omega, t|\vec{x}_0)dt. \tag{2.12}$$

Since $S(\partial\Omega, 0|\vec{x}_0) = 1$ forall $\vec{x}_0 \in Int(\Omega)$, $\lim_{t\to 0} t^m S(\partial\Omega, t|\vec{x}_0) = 0$. As in the $d = 1$ case one has to be careful about the value at the other extreme. Clearly $S(\partial\Omega, 0|\vec{x}_0) \to 0$ as $t \to \infty$ but, in order to have a well defined moment of order m we have to ask that, for fixed m, $S(\partial\Omega, t|\vec{x}_0) \sim 1/t^{m+\epsilon}$ as $t \to \infty$. In this case $\lim_{t\to\infty} t^m S(\partial\Omega, t|\vec{x}_0) = 0$ and

$$\boxed{T^{(m)}(\partial\Omega, \vec{x}_0) = m\int_0^\infty t^{m-1}S(\partial\Omega, t|\vec{x}_0)dt.} \tag{2.13}$$

In particular, for the MFPT we have

$$\boxed{T^{(1)}(\partial\Omega, \vec{x}_0) = \int_0^\infty S(\partial\Omega, t|\vec{x}_0)dt.} \tag{2.14}$$

As for the $d = 1$ case we limit ourselves to Markov, continuous Gaussian processes where the conditional probabiity density $p(\vec{x}, t|\vec{x}_0, 0)$ satisfies the Fokker-Planck equation

$$\frac{\partial}{\partial t}p(\vec{x}, t|\vec{x}_0, 0) = \hat{L}_{FP}(\vec{x}, t)p(\vec{x}, t|\vec{x}_0, 0) \tag{2.15}$$

or in its continuity form

$$\frac{\partial}{\partial t}p(\vec{x}, t|\vec{x}_0, 0) + \nabla\cdot\vec{j}(\vec{x}, t|\vec{x}_0, 0) = 0. \tag{2.16}$$

Sometimes it is useful to express $T^{(1)}(\partial\Omega, \vec{x}_0)$ in terms of the current density. This is easily done by integrating both terms of the continuity equation on Ω:

$$\frac{\partial}{\partial t} S(t, |\vec{x}_0) = -\int_\Omega \nabla \cdot \vec{j}(\vec{x}, t|\vec{x}_0, 0) d\vec{x} = \int_{\partial\Omega} \vec{j}(\vec{x}, t|\vec{x}_0, t_0) \cdot \hat{n} dS. \tag{2.17}$$

This gives

$$T^{(1)}(\partial\Omega, \vec{x}_0) = -\int_0^\infty t \frac{\partial}{\partial t} S(\partial\Omega, t|\vec{x}_0) dt = \int_0^\infty t \left[\int_{\partial\Omega} \vec{j}(\vec{x}, t|\vec{x}_0, t_0) \cdot \hat{n} dS \right] dt \tag{2.18}$$

2.0.1 PDE for the evolution of $S(\partial\Omega, t|\vec{x}_0)$

The procedure to find the evolution equation for $S(\partial\Omega, t|\vec{x}_0)$ in $d > 1$ is a simple generalization of the one presented above for the $d = 1$ case. Let us here describe it in more detail for the following d dimensional Fokker Planck operator:

$$\hat{L}_{FP}(\vec{x}) = \nabla \cdot D(\vec{x})\nabla + \beta\nabla \cdot D(\vec{x})(\nabla U(\vec{x}) \tag{2.19}$$

where $U(\vec{x})$ is a generic potential. The first step consists in computing the adjoint operator of $\hat{L}_{FP}(\vec{x})$. We do it here explicitely. For some test function $u(\vec{x})$ and $v(\vec{x})$ we have

$$\begin{aligned}
\int_\Omega v(\vec{x})\hat{L}_{FP}(\vec{x})u(\vec{x}) &= \int_\Omega v(\vec{x}) \left[\nabla \cdot D(\vec{x})\nabla\right] u(\vec{x}) d\vec{x} + \beta \int_\Omega v(\vec{x}) \left[\nabla \cdot D(\vec{x})(\nabla U)\right] u(\vec{x}) d\vec{x} \\
&= \int_\Omega \nabla \cdot \left[v(\vec{x})D(\vec{x})\nabla u(\vec{x})\right] d\vec{x} - \int_\Omega \nabla \cdot v(\vec{x}) \left[D(\vec{x})\nabla u(\vec{x})\right] d\vec{x} \\
&+ \beta \int_\Omega \nabla \cdot \left[v(\vec{x})D(\vec{x})(\nabla U)u(\vec{x})\right] d\vec{x} - \beta \int_\Omega \nabla \cdot v(\vec{x}) \left[D(\vec{x})(\nabla U)u(\vec{x})\right] d\vec{x} \\
&= \int_\Omega \nabla \cdot \left[v(\vec{x})D(\vec{x})\nabla u(\vec{x})\right] d\vec{x} - \int_\Omega \nabla \cdot \left[D(\vec{x})\nabla \cdot v(\vec{x})u(\vec{x})\right] d\vec{x} \\
&+ \int_\Omega \nabla \cdot \left[D(\vec{x})\nabla v(\vec{x})\right] u(\vec{x}) d\vec{x} + \beta \int_\Omega \nabla \cdot \left[v(\vec{x})D(\vec{x})(\nabla U)u(\vec{x})\right] d\vec{x} \\
&- \beta \int_\Omega \left[D(\vec{x})(\nabla U)\right] \nabla \cdot v(\vec{x})u(\vec{x}) d\vec{x}
\end{aligned} \tag{2.20}$$

Since this is true for any test function one can formally write

$$v\hat{L}_{FP}u - u\hat{L}^\dagger v = \nabla \cdot P[u, v], \tag{2.21}$$

where

$$\hat{L}^\dagger(\vec{x}) = \nabla \cdot D(\vec{x})\nabla - \beta D(\vec{x})(\nabla U) \cdot \nabla \tag{2.22}$$

and the bilinear form

$$P[u, v] = vD\nabla u - uD\nabla v + \beta D(\nabla U)uv. \tag{2.23}$$

For a given Fokker-Planck operator, the formal solution of the FP equation is given by

$$p(\vec{x}, t|\vec{x}_0, t_0) = \int_\Omega \delta(\vec{x} - \vec{x}') e^{t\hat{L}_{FP}(\vec{x}')} \delta(\vec{x}' - \vec{x}_0) d\vec{x}' \tag{2.24}$$

Since $P[\delta(\vec{x} - \vec{x}'), \delta(\vec{x}' - \vec{x}_0)]$ for $\vec{x}$ and $\vec{x}_0$ inside the region Ω vanishes on $\partial\Omega$ one can rewrite the solution 2.24 as

$$p(\vec{x}, t|\vec{x}_0, t_0) = \int_\Omega \delta(\vec{x}' - \vec{x}_0) e^{t\hat{L}^\dagger_{FP}(\vec{x}')} \delta(\vec{x} - \vec{x}') d\vec{x}'. \tag{2.25}$$

Differentiating the last equation with respect to t yields the *backward Fokker-Planck* equation [1]

$$\partial_t p(\vec{x}, t|\vec{x}_0, t_0) = \hat{L}^\dagger(\vec{x}_0) p(\vec{x}, t|\vec{x}_0, t_0). \tag{2.26}$$

[1] The Backward Fokker-Planck equation can be also obtained directly starting from the Chapmann-Kolmogorov equation. See Chapter on Fokker-Planck TODO

Equation (2.26) has to be complemented by BC which garantee $P[u, v]$ to vanish on $\partial\Omega$. This requires eq. (2.23) to vanish on $\partial\Omega$. If we identify u and v with the solution of Eqs. (2.24) and (**??**) respectively one has to require, in the case for example of the absorbing condition on Γ_{in}: $p(\vec{x} \in \Gamma_{in}, t) = 0$, $u(x \in \Gamma_{in}) = 0$ and $v(\vec{x} \in \Gamma_{in}) = 0$, i.e. $(D(\vec{x} \in \Gamma_{in}) \neq 0)$,

$$p(\vec{x}, t|\vec{x}_0, 0) = 0, \qquad \vec{x}_0 \in \Gamma_{in}. \tag{2.27}$$

In the case of *radiation boundary condition* (or Robin BC) at Γ_{in}

$$j(\vec{x} \in \Gamma_{in}, t) = kp(\vec{x} \in \Gamma_{in}, t), \tag{2.28}$$

$\nabla u + \beta(\nabla U)u = [k/D(\vec{x} \in \Gamma_{in})]u$, we have $\nabla v = [k/D(\vec{x} \in \Gamma_{in})]v$, i.e, $[D(\vec{x} \in \Gamma_{in}) \neq 0]$,

$$\nabla_{\vec{x}_0} p(\vec{x}, t|\vec{x}_0, 0) = \frac{k}{D(\vec{x}_0)} p(\vec{x}, t|\vec{x}_0, 0), \qquad \vec{x}_0 \in \Gamma_{in}. \tag{2.29}$$

At this point we can derive a PDE for the survival probability $S(\partial\Omega, t, |\vec{x}_0)$ by simply integrating eq. (2.26) over $\vec{x}$. This gives

$$\partial_t S(\partial\Omega, t|\vec{x}_0) = \hat{L}^\dagger(\vec{x}_0) S(\partial\Omega, t|\vec{x}_0). \tag{2.30}$$

The boundary conditions (**??**) and (2.28) become respectively $[D(\vec{x} \in \Gamma_{in}) \neq 0]$,

$$S(\partial\Omega, t|\vec{x}_0) = 0 \qquad \vec{x}_0 \in \Gamma_{in}, \tag{2.31}$$

and

$$\nabla S(\partial\Omega, t|\vec{x}_0) = \frac{k}{D(\vec{x}_0)} S(\partial\Omega, t|\vec{x}_0) \qquad \vec{x}_0 \in \Gamma_{in}. \tag{2.32}$$

2.0.2 ODE for the MFPT

As for the $d = 1$, to obtain a differential equation for $T^{(1)}(\partial\Omega, \vec{x}_0)$ it is sufficient to integrate eq. (2.30) over time. Since

$$\int_{\mathbb{R}^+} (\partial/\partial t) S(\partial\Omega, t|\vec{x}_0) = S(\partial\Omega, \infty|\vec{x}_0) - S(\partial\Omega, 0|\vec{x}_0) = -1, \tag{2.33}$$

we finally have

$$\boxed{\hat{L}^\dagger_{FP}(\vec{x}_0) T^{(1)}(\vec{x}_0) = -1.} \tag{2.34}$$

In general it is not simple to solve analytically either the Fokker-Planck equation in any dimensions and get $p(\vec{x}, t|\vec{x}_0, 0)$ or solve the PDE (2.30) for $S(\partial\Omega, 0|\vec{x}_0)$ or even the ODE (2.34) for the MFPT. In some particular cases, however, it is possible to reach some level of knowledge from analytical computation. Below we present some of these cases that mainly relies on symmetric properties of the problem.

2.0.3 MFPT for symmetric diffusion in d dimensions

In this case the stochastic process $\vec{X}(t)$ is a simple free diffusion. Let us see how the MFPT can be computed by following the 3 different routes mentioned in the previous chapter.

MFPT from route [i]

In this full approach we start from the solution of $p(r, t|r_0, t)$ found for spherical symmetric free diffusion where the boundary at $a = R_{in}$ is absorbing. Recalling Eq. (**??**) and putting $a = R_{in}$ we have

$$p(r, t|r_0, t_0) = \frac{1}{4\pi r r_0} \frac{1}{\sqrt{4\pi D(t - t_0)}} \left(\exp\left[-\frac{(r - r_0)^2}{4D(t - t_0)} \right] - \exp\left[-\frac{(r + r_0 - 2R_{in})^2}{4D(t - t_0)} \right] \right). \tag{2.35}$$

We recall (see beginning of the chapter) that in general, given $p(\vec{r}, t|\vec{r}_0, t_0)$ the reaction rate can be obtained as

$$w(t|\vec{r}_0, t_0) = -\frac{d}{dt}S(t|\vec{r}_0) = -\partial_t \int_\Omega \nabla \cdot \vec{j}(\vec{r}, t|\vec{r}_0, t_0)d\vec{r} = \int_{\partial\Omega} \vec{j} \cdot \hat{n} dS \tag{2.36}$$

In our case $\partial\Omega = \Gamma_1$ and being the problem spherical symmetric, we have

$$w(t|r_0, t_0) = 4\pi R_{in}^2 D\partial_r p(r, t|r_0, t_0) \mid_{r=R_{in}} \tag{2.37}$$

where the factor $4\pi R_{in}^2$ takes the surface area of the spherical boundary into account. By inserting (2.35) into (2.37) one gets

$$w(t|r_0, t_0) = \frac{R_{in}}{r_0} \frac{1}{\sqrt{4\pi D(t-t_0)}} \frac{r_0 - R_{in}}{t - t_0} \exp\left[-\frac{(r_0 - R_{in})^2}{4D(t-t_0)}\right]. \tag{2.38}$$

From the reaction rate $w(t|r_0, t_0)$ one can evaluate the fraction of particles which react at the boundary $r = R_{in}$ according to

$$N_{react}(t|r_0, t_0) = \int_{t_0}^{t} w(t'|r_0, t_0)dt'. \tag{2.39}$$

MFPT from route [ii]

In this approach the idea is to solve the Backward equation for the survival probability, i.e.

$$\frac{\partial}{\partial_t} S(t|\vec{r}_0) = \hat{L}^\dagger(\vec{r}_0)S(t|\vec{r}_0) \tag{2.40}$$

where, we recall here,

$$\hat{L}^\dagger(\vec{r}_0) = \vec{\nabla} \cdot D(\vec{r})\vec{\nabla} - \beta D(\vec{r})\left(\vec{\nabla}U\right) \cdot \vec{\nabla} \tag{2.41}$$

and the Robin BC

$$\nabla S(t|\vec{r}_0) = \frac{k}{D(\vec{r}_0)} S(t|\vec{r}_0) \qquad r_0 \in \Gamma_1. \tag{2.42}$$

If we assume a perfect spherical symmetry for $D(\vec{r})$ and $U(\vec{r})$, the backward FP equation simplifies (in d dimensions) to

$$\frac{\partial}{\partial t} S(t|r_0) = \frac{\partial}{\partial r_0} D(r_0) \frac{\partial}{\partial r_0} S(t|r_0) + D(r_0)\left[\frac{d-1}{r_0} - \beta\frac{dU}{dr_0}\right] \frac{\partial}{\partial r_0} S(t|r_0). \tag{2.43}$$

The radiative BC in Γ_1 simplifies to:

$$\left.\frac{\partial}{\partial r_0} S(t|r_0)\right|_{r_0=R_{in}} = \frac{k}{D(R_{in})} S(t|R_{in}). \tag{2.44}$$

The outer boundary condition can be taken to be

$$\lim_{r_0 \to \infty} S(t|r_0) = 1 \tag{2.45}$$

or reflecting , if Γ_2 is bounded,

$$\left.\frac{\partial}{\partial r_0} S(t|r_0)\right|_{r_0=R_{ext}} = 0. \tag{2.46}$$

Clearly, the initial condition is

$$S(0|r_0) = 1, \tag{2.47}$$

since at $t = 0$ the particle has not reached any boundary yet. In order to simplify the above problem let us consider a constant diffusion equation: $D(r_0) = D$. A possible way to get $S(t|r_0)$ is to compute first the Laplace transform

$$\tilde{S}(s|r_0) = \int_{\mathbb{R}^+} e^{-st} S(t|r_0) \tag{2.48}$$

and then perform (whenever is possible) the inverse trasform to get back $S(t|r_0)$. The equation for $\tilde{S}(s|r_0)$ becomes

$$D\left[\frac{d^2}{dr_0^2}\tilde{S}(s|r_0) + \left(\frac{d-1}{r_0} - \beta\frac{dU}{dr_0}\right)\right] = s\tilde{S}(s|r_0) - S(t=0|r_0) \tag{2.49}$$

TODO

It is interesting to note that the survival probabilities calculated using different reactive boundary conditions are related,as they are solution of the same partial differential equation. Indeed it easy to show (Exercise) that

$$s\tilde{S}_{rad}(s|r_0) = 1 - \frac{1 - s\tilde{S}_{abs}(s|r_0)}{1 + DR_{in}^{d-1}(s/k)(\partial\tilde{S}_{abs}(s|r_0)/\partial r_0)_{r=R_{in}}} \tag{2.50}$$

MFPT from route [iii]

Eq. (**??**) can be solved analytically not only for few problems in $d = 1$ but also for any d where the boundary conditions, the potential, and the diffusion coefficient in an orthogonal curvilinear coordinate system depend solely on a single coordinate. In particular, for d dimensions employing spherical coordinates and exployting spherical symmetry we have

$$r_0^{1-d}\frac{d}{dr_0}\left[r_0^{d-1}D(r_0)\frac{d}{dr_0}T^{(1)}(r_0)\right] - D(r_0)\beta\frac{dU}{dr_0}\frac{d}{dr_0}T^{(1)}(r_0) = -1. \tag{2.51}$$

Suppose that Γ_{in} and Γ_{ext} are spherical surfaces respectively of radius R_{in} and R_{ext} with $R_{in} < R_{ext}$. In this case absorbing boundary conditions correspond to

$$T^{(1)}(r_0 = R_{in}) = T^{(1)}(r_0 = R_{ext}) = 0 \tag{2.52}$$

reflecting BC to

$$\left[\frac{d}{dr_0}T^{(1)}(r_0)\right]_{r_0=R_{in}} = \left[\frac{d}{dr_0}T^{(1)}(r_0)\right]_{r_0=R_{ext}} = 0 \tag{2.53}$$

and radiation BC, say at $r_0 = R_{in}$ to

$$\left[\frac{d}{dr_0}T^{(1)}(r_0)\right]_{r_0=R_{in}} = \frac{k}{D(R_{in})}T^{(1)}(R_{in}). \tag{2.54}$$

A classical problem correspond to the case in which the bigger surface is the container (cell) whereas the inner sphere describes a target. In this respect the correct BC to impose are reflecting on Γ_{ext} and radiating on Γ_{in}:

$$\left[\frac{d}{dr_0}T^{(1)}(r_0)\right]_{r_0=R_{ext}} = 0 \tag{2.55}$$

$$\left[\frac{d}{dr_0}T^{(1)}(r_0)\right]_{r_0=R_{in}} = \frac{k}{D(R_{in})}T^{(1)}(R_{in}). \tag{2.56}$$

Since Eq. (2.51) corresponds to a first-order inhomogeneous ODE it can be easily solved subject to the above BC. This gives

$$T^{(1)}(r_0) = \int_{R_{in}}^{r_0} \frac{\rho_1^{1-d}}{D(\rho_1)} e^{\beta U(\rho_1)} d\rho_1 \int_{\rho_1}^{R_{ext}} \rho_2^{d-1} e^{-\beta U(\rho_2)} d\rho_2 + \frac{1}{k} R_{in}^{1-d} e^{\beta U(R_{in})} \int_{R_{in}}^{R_{ext}} \rho_2^{d-1} e^{-\beta U(\rho_2)} d\rho_2. \quad (2.57)$$

Note that in the $k \to \infty$ limit corresponding to pure absorbing BC at $r_0 = R_{in}$ the second term of eq. (2.57) vanishes. In the opposite limit $k \to 0$ (almost reflecting BC), is the second term that dominates the statistics and $T^{(1)}(r_0)$ is essentially independent on r_0:

$$T^{(1)} \sim \frac{1}{k} R_{in}^{1-d} e^{\beta U(R_{in})} \int_{R_{in}}^{R_{ext}} \rho_2^{d-1} e^{-\beta U(\rho_2)} d\rho_2. \quad (2.58)$$

So far we have considered the general case in which a potential $U(r)$ is present. Now we simplify the problem by looking at free diffusion $U(r) = 0$. In this case Eq. (2.57) simplifies to

$$T^{(1)}(r_0) = \int_{R_{in}}^{r_0} \frac{\rho_1^{1-d}}{D(\rho_1)} d\rho_1 \int_{\rho_1}^{R_{ext}} \rho_2^{d-1} d\rho_2 + \frac{1}{k} R_{in}^{1-d} \int_{R_{in}}^{R_{ext}} \rho_2^{d-1} d\rho_2 \quad (2.59)$$

In the simpler case of $D(r_0) = D$ we have:

$$T^{(1)}(r_0) = \frac{1}{D} R_{ext}(r_0 - R_{in}) - \frac{1}{2D}(r_0^2 - R_{in}^2) + \frac{R_{ext} - R_{in}}{k} \qquad d = 1; \quad (2.60)$$

$$T^{(1)}(r_0) = \frac{R_{ext}^2}{2D} \ln(r_0/R_{in}) - \frac{R_{in}^2}{4D} \left(\left(\frac{r_0}{R_{in}} \right)^2 - 1 \right) + \frac{R_{ext}}{2k} \left(\frac{R_{ext}}{R_{in}} - \frac{R_{in}}{R_{ext}} \right) \qquad d = 2 \quad (2.61)$$

and

$$T^{(1)}(r_0) = \frac{R_{ext}^3}{3D} \left(R_{in}^{-1} - r_0^{-1} \right) - \frac{1}{6D} \left(r_0^2 - R_{in}^2 \right) + \frac{1}{3kR_{in}^2} \left(R_{ext}^3 - R_{in}^3 \right) \qquad d = 3. \quad (2.62)$$

To obtain the MFPT we should average over the initial position r_0. Suppose for example that the particles start at the spherical surface Γ_2 with $r_0 = R_{ext}$. This means $f_0(r_0) = \delta(r_0 - R_{ext})$. Hence $T^{(1)} = \int_{R_{in}}^{R_{ext}} T^{(1)}(r_0)\delta(r_0 - R_{ext})$ and in the 3 cases above this gives

$$\frac{T^{(1)} D}{R_{ext}^2} = \frac{1}{2}(x - 10^2 + \frac{D}{R_{ext} k}(1 - x) \qquad d = 1; \quad (2.63)$$

$$\frac{T^{(1)} D}{R_{ext}^2} = \frac{1}{4}(x^2 - 1) - \frac{\ln x}{2} + \frac{1}{2kR_{ext}x}(1 - x^2) \qquad d = 2; \quad (2.64)$$

$$\frac{T^{(1)} D}{R_{ext}^2} = \frac{1}{6}(x^2 - 1) + \frac{1}{3}\left(1 - \frac{1}{x}\right) + \frac{D}{3kR_{ext}x^2}(1 - x^3) \qquad d = 3 \quad (2.65)$$

where $x = R_{in}/R_{ext}$.