MASTER THESIS

A model of non-interacting particles in one dimension under resetting dynamics

International Master Course in Physics of Complex Systems

Supervisor:
Prof. Satya Majumdar

Co-Supervisor:
Prof. Alessandro Pelizzola

Candidato:
Costantino Di Bello

Anno Accademico 2020/2021

Contents

Introduction

When you are asked by yours to find something in the house it could take centuries to find them. A common strategy is to search unsuccessfully for a while, then restart the search from the starting point (finally give it up failing the task and being rebuked since it was just in front of your eyes). Also when we search for a face in a crowd we tend to use the same strategy till we get the target. Resetting seems to be a very natural way of searching.
In general, search processes are ubiquitous both in human behavior and in nature: let us think about animals or bacteria searching for food, or biomolecules searching for binding sites, et similia. In these contexts resetting turned out to be very advantageous, and scientific literature is full of these examples. Also in computer science (and I am not referring to the famous trick of switching computer off and on) resetting has been widely exploited, like in stochastic algorithms or in simulating dynamics of free energy landscapes.

As we will see in next chapters, adding a resetting rate to a certain dynamics generally leads to the appearance of a non-equilibrium steady state (NESS). A paradigmatic example has been discussed in [3]. Although this thesis tries to be self-consistent, a prior knowledge on the topic can be very helpful. A quite exhaustive reading on resetting processes is [5], which contains a lot of results on the topic and many references for further readings.

For what concerns this thesis, the work is organized as follows: in the first chapter we will review some famous results useful for further discussions; in second chapter we will discuss a model of non-interacting particles with resetting on a line; in the third and last chapter we will see how to simulate the system in order to verify if analytical results are correct.

Chapter 1

Preliminary tools

In this chapter we will expose some equations and tools of the field which will be useful in the following sections. We will mainly refer to standard references on stochastic processes [6] and to the literature on resetting [5] which contain essentially all the instruments we need.

1.1 Fokker-Planck equations with resetting

1.1.1 Diffusion with resetting

Fokker-Planck (FP) equation is a very general method to describe the time evolution of the probability density. For a particle performing a Brownian motion in a one-dimensional space, the Fokker-Planck equation describing the motion is [6]

$$\frac{\partial p(x,t \mid x_0)}{\partial t} = D\frac{\partial^2 p(x,t \mid x_0)}{\partial x^2}, \tag{1.1}$$

where D is the diffusivity constant $[D] = s^2 t^{-1}$, and $p(x,t \mid x_0)$ is the probability of having a particle in x at time t given that it started in x_0 at time $t = 0$[1]. Our aim is now to derive FP equation for Brownian motion with resetting.
We will consider a Poissonian resetting rate r[2], which means that in an infinitesimal time interval dt only a resetting event is possible and the probability of its

[1] FP equation can be also interpreted in this way which is maybe easier to understand: we could imagine a swarm of explorers in a certain phase space each one performing the same Brownian dynamics, then the FP equation describes the density of searchers in a certain position at a given time.

[2] For the following discussion there is no need to enter in mathematical details on Poissonian processes, hence we will expose a less rigorous but more physical treatment. Notice that from now on we will always refer to Poissonian resetting.

occurrence is rdt. Therefore the position of the searcher is updated according to the stochastic rule [5]

$$x(t+dt) = \begin{cases} X_r & \text{with probability } rdt \\ x(t) + \xi(t)\sqrt{dt} & \text{with probability } 1 - rdt \end{cases} \tag{1.2}$$

where we indicate with X_r the resetting position (in principle different from the initial position x_0), with $\xi(t)$ a Gaussian random variable with 0 mean and variance $2D$

$$\langle \xi(t) \rangle = 0 \quad \text{and} \quad \langle \xi(t)\xi(t') \rangle = 2D\delta(t-t'). \tag{1.3}$$

A possible trajectory is sketched in the next figure

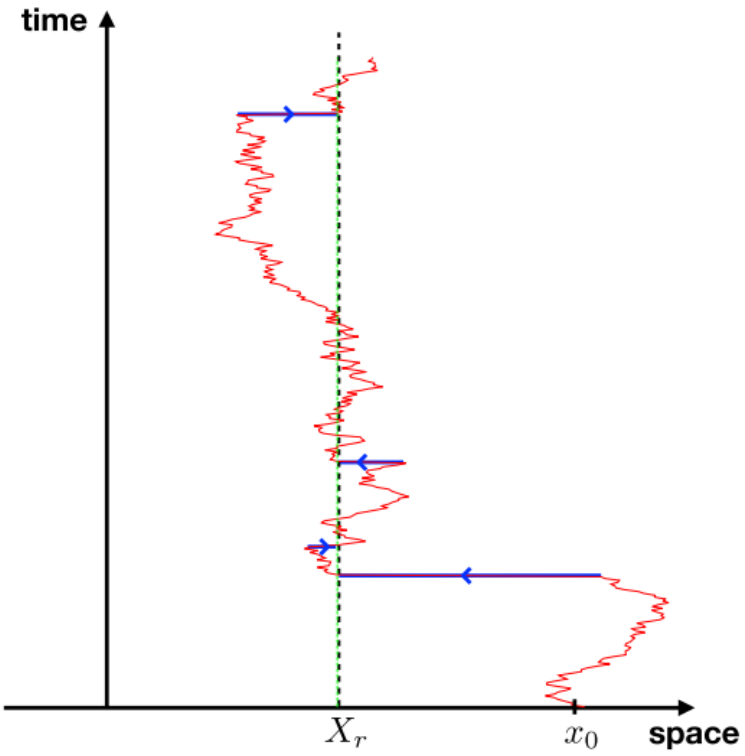

Figure 1.1: The figure is taken from [5]. A particle starting in x_0 performing a diffusive dynamics with resetting on X_r.

The meaning of the system is evident: the particle can either reset in the time interval dt with probability rdt, or diffuse with probability $1 - rdt$. Considering discrete and infinitesimal time and space steps dt and dx, the forward master equation of the system writes:

$$p(x, t + \mathrm{d}t \mid x_0, X_r) = r\mathrm{d}t\delta\left(x - X_r\right) + (1 - r\mathrm{d}t)\int_{-\infty}^{+\infty} \mathcal{D}\xi \; p\left(x - \xi\sqrt{\mathrm{d}t}, t \mid x_0, X_r\right) \tag{1.4}$$

at the right hand side (rhs) the first term represents a probability flux due to resetting, while the second term considers all possibilities arising in the case no resetting event occurred. Hence the integral $\int \mathcal{D}\xi$ weights all possible realization of the noise. Dropping the conditioning on x_0 and X_r to make the notation more concise, and expanding the above expression in dt we get

$$\begin{aligned} p(x, t + \mathrm{d}t) &= r\mathrm{d}t\delta\left(x - X_r\right) + \\ &+ (1 - r\mathrm{d}t)\int_{-\infty}^{+\infty} \mathcal{D}\xi \left[p(x,t) - \sqrt{dt}\xi(t)\frac{\partial p(x,t)}{\partial x} + dt\frac{\xi^2(t)}{2}\frac{\partial^2 p(x,t)}{\partial x^2} + \dots\right]. \end{aligned} \tag{1.5}$$

Performing the integration keeping in mind (1.3) and taking the limit $\mathrm{d}t \to 0$ we obtain:

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2} - rp(x,t) + r\delta(x - X_r), \tag{1.6}$$

with the initial condition $p(x, 0) = \delta(x - x_0)$. In the following we will always consider the case in which the resetting position coincides with the initial position, i.e. $X_r = x_0$.

1.1.2 Some observations on diffusive dynamics with resetting

For a diffusive motion in an unbounded domain a stationary solution does not exist. Indeed, the limit for $t \to \infty$ of the formula[3]

$$p_0(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x - x_0)^2}{4Dt}\right) \tag{1.7}$$

which is the solution of the simple diffusion equation, is vanishing.
While, the stationarity for equation (2.1), which reads

$$D\frac{\partial^2 p_r(x)}{\partial x^2} - rp_r(x) + r\delta(x - x_0) = 0 \tag{1.8}$$

[3]From now on our notation will use the subscript to denote the resetting rate, hence p_0 will be the Green function in the case without resetting.

has a non-vanishing solution of a Laplacian shape around the resetting position:

$$p_r(x) = \frac{1}{2}\sqrt{\frac{r}{D}} \exp\left(-\sqrt{\frac{r}{D}}|x - x_0|\right). \tag{1.9}$$

In general, indeed, adding a resetting rate to a certain dynamics leads, since detailed balance clearly does not hold due to the presence of a constant flux towards resetting position, to the emergence of a non-equilibrium stationary state (NESS). An interesting discussion on how the NESS is reached is exposed in [10]. The study of how the NESS is reached will be also exposed in this text and will be crucial for some further discussions.

1.2 Renewal approach to solve the Fokker-Planck equation

This section shows a very general tecnique to find the Green function $p_r(x, t \mid x_0)$ of a resetting process. To compute the quantity $p_r(x, t \mid x_0)$ we have to consider two contributions: one coming from trajectories in which no resetting occurred up to time t, and the other from trajectories in which some resetting occurred. Therefore:

$$p_r(x, t \mid x_0) = e^{-rt} p_0(x, t \mid x_0) + r \int_0^t \mathrm{d}\tau e^{-r\tau} p_0(x, \tau \mid X_r) \tag{1.10}$$

Where the Green function of the simple diffusion p_0 is weighted, in the first term, with e^{-rt} (absence of resetting up to time t), while in the second term is multiplied by $re^{-r\tau}$, which is the probability that last resetting event occurred at time $t - \tau$, integrated over all possible values of τ. The previous equation goes under the name of *last renewal equation*, analogously we could also write a *first renewal equation*:

$$p_r(x, t \mid x_0) = e^{-rt} p_0(x, t \mid x_0) + r \int_0^t \mathrm{d}\tau e^{-r\tau} p_0(x, t - \tau \mid X_r) \tag{1.11}$$

whose interpretation should now be clear from previous considerations[4]
Interestingly both last and first renewal equations do not depend on the dynamics (just a Poissonian resetting rate is required to make they hold).

1.3 Green functions for various processes

In this section we will derive some important results (already found in literature) which will be widely used in following sections.

[4]The equivalence between first and last renewal equation can be simply proven by means of Laplace transform. See appendix of [5].

1.3.1 Diffusion with resetting

For this case we already have an expression for the Green function, for instance following equation (1.10) in the case $X_r = x_0$:

$$p_r(x,t \mid x_0) = \frac{e^{-rt}}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) + r\int_0^t \frac{e^{-r\tau}}{\sqrt{4\pi D\tau}} \exp\left(-\frac{(x-x_0)^2}{4D\tau}\right) \mathrm{d}\tau \tag{1.12}$$

Nevertheless it is convenient, for further manipulations, to proceed in an another way. We will apply Laplace transform to equation (2.1). Hence, exploiting the following definition

$$\tilde{p}_r(x,s \mid x_0) = \int_0^{+\infty} e^{-st} p_r(x,t \mid x_0)\mathrm{d}t \tag{1.13}$$

and observing that the second term in (2.1) can be seen as a convolution between 1 and $e^{-r\tau}p_0(x,\tau \mid x_0)$, we get

$$\tilde{p}_r(x,s \mid x_0) = \tilde{p}_0(x,r+s \mid x_0) + \frac{r}{s}\tilde{p}_0(x,r+s \mid x_0) \tag{1.14}$$

$$\text{thus} \quad \tilde{p}_r(x,s \mid x_0) = \frac{r+s}{s}\, \tilde{p}_0(x,r+s \mid x_0). \tag{1.15}$$

The function $\tilde{p}_0(x,s \mid x_0)$ can be obtained through the definition (1.13)

$$\begin{aligned}\tilde{p}_0(x,s \mid x_0) &= \int_0^{+\infty} \frac{e^{-s\tau}}{\sqrt{4\pi D\tau}} \exp\left(-\frac{(x-x_0)^2}{4D\tau}\right) \mathrm{d}\tau \\ &= \frac{1}{\sqrt{4Ds}} \exp\left(\sqrt{\frac{s}{D}}|x-x_0|\right),\end{aligned} \tag{1.16}$$

where we used a result shown in [13, Table of Laplace transforms]. Finally, inserting the last result in equation (1.15), we obtain

$$\tilde{p}_r(x,s \mid x_0) = \frac{1}{\sqrt{4D}} \frac{\sqrt{r+s}}{s} \exp\left(-\sqrt{\frac{r+s}{D}}\ |x-x_0|\right). \tag{1.17}$$

1.3.2 Run-and-tumble particles

Case without resetting For the sake of clarity, we will expose the case without resetting first and then we will add, as usual, a Poissonian resetting rate.

Run-and-tumble particles (RTP) are very frequently used in active matter and stochastic processes literature. This kind of dynamics has been used to model the motion various species of bacteria. The Langevin equation for this dynamics is:

$$\frac{dx}{dt} = v_0\sigma(t) \tag{1.18}$$

Where v_0 is the intrinsic speed during a run, $\sigma(t) = \pm 1$ is a telegraphic noise. Essentially the particle moves in a specific direction with constant velocity till the occurrence of a tumbling. The tumbling event, occurring with a fixed rate γ, reverses the direction of motion (of course are referring to one-dimensional case). Let be $\xi(t) = v_0\sigma(t)$, as shown in [1] we have the following relations:

$$\begin{aligned}\langle \xi(t)\xi(t')\rangle &= v_0^2 e^{-2\gamma|t-t'|} \\ &= \frac{v_0^2}{\gamma}\left[\gamma e^{-2\gamma|t-t'|}\right]\end{aligned} \tag{1.19}$$

hence taking the limit $v_0 \to +\infty$, $\gamma \to +\infty$, with $\frac{v_0^2}{\gamma} = constant$ we get a relation of the same form of (1.3):

$$\langle \xi(t)\xi(t')\rangle \to 2D_{\text{eff}}\delta(t-t') \tag{1.20}$$

where we set $D_{\text{eff}} = v_0^2/2\gamma$. This property, usually called *diffusive limit*, is quite general and constitutes a kind of 'sanity check' for calculations on RTP (we will come back on this idea later).

To find the Green function of the system we can use, as before, the formalism of master equation. But nonetheless, at variance with the diffusive case, here we will have a system of forward master equations (the derivation follows [4])

$$\frac{\partial p_+(x,t)}{\partial t} = -v_0\frac{\partial p_+(x,t)}{\partial x} + \gamma p_-(x,t) - \gamma p_+(x,t), \tag{1.21}$$

$$\frac{\partial p_-(x,t)}{\partial t} = +v_0\frac{\partial p_-(x,t)}{\partial x} + \gamma p_+(x,t) - \gamma p_-(x,t), \tag{1.22}$$

where $p_\pm(x,t)$ is the probability of having velocity $\pm v_0$ and be at position x at time t. As we can see there are two terms multiplied to γ for each equation, they both represents a probability 'gain' or 'loss' due to tumbling. To solve the system we make use of Laplace transform, so we define

$$\tilde{p}_\pm(x,s) = \int_0^{+\infty} e^{-st}p_\pm(x,t)\mathrm{d}t. \tag{1.23}$$

Taking the Laplace transform of equation (1.21),(1.22) we obtain

$$-p_+(x,0) + v_0\frac{\partial \tilde{p}_+}{\partial x} + (s+\gamma)\tilde{p}_+ - \gamma\tilde{p}_- = 0; \tag{1.24}$$

$$-p_-(x,0) - v_0\frac{\partial \tilde{p}_+}{\partial x} + (s+\gamma)\tilde{p}_- - \gamma\tilde{p}_+ = 0. \tag{1.25}$$

For simplicity we set as initial condition to be at the origin (we could simply apply a translation if initial position is different), with equal probability in the choice of initial direction, i.e. $P_+(x,0) = P_-(x,0) = \frac{1}{2}\delta(x)$. Thus, far from origin, we have

$$\tilde{p}_- = \frac{v_0}{\gamma}\frac{\partial \tilde{p}_+}{\partial x} + \frac{s+\gamma}{\gamma}\tilde{p}_+ \tag{1.26}$$

$$\tilde{p}_+ = -\frac{v_0}{\gamma}\frac{\partial \tilde{p}_-}{\partial x} + \frac{s+\gamma}{\gamma}\tilde{p}_- \tag{1.27}$$

by very simple algebra we obtain

$$v_0^2\frac{\partial^2 \tilde{p}_\pm}{\partial x^2} - \left[(s+\gamma)^2 - \gamma^2\right]\tilde{p}_\pm = 0, \tag{1.28}$$

which has a simple solution (taking only non-diverging exponentials)

$$\begin{array}{lll} \tilde{p}_\pm = A_\pm \mathrm{e}^{-\lambda x} & \text{for} & x > 0 \\ \tilde{p}_\pm = B_\pm \mathrm{e}^{+\lambda x} & \text{for} & x < 0 \end{array} \tag{1.29}$$

with

$$\lambda(s) = \left(\frac{s(s+2\gamma)}{v_0^2}\right)^{1/2}. \tag{1.30}$$

By simply substituting this result in equations (1.24),(1.25) we get the conditions

$$(s+\gamma-\lambda v_0)\,A_+ = \gamma A_- \tag{1.31}$$

$$(s+\gamma+\lambda v_0)\,B_+ = \gamma B_- \tag{1.32}$$

Moreover, by continuity in $x = 0$, we also have the relation

$$A_+ + A_- = B_+ + B_-. \tag{1.33}$$

Finally, the normalization condition imposes

$$\int \mathrm{d}x\,[\tilde{p}_+ + \tilde{p}_-] = \frac{1}{s}, \tag{1.34}$$

which implies

$$A_+ + A_- = B_+ + B_- = \frac{\lambda}{2s}, \tag{1.35}$$

and therefore

$$\tilde{p}(x,s) = \tilde{p}_+(x,s) + \tilde{p}_-(x,s) = \frac{\lambda}{2s} e^{-\lambda|x|} \tag{1.36}$$

where λ is given by relation (1.30).
Using the Laplace inversion formula

$$p(x,t) = \left(\mathcal{L}^{-1}\tilde{p}(x,s)\right)(t) = \int_\Gamma \frac{ds}{2\pi i} e^{st} \frac{\lambda(s)}{2s} e^{-\lambda(s)|x|} \tag{1.37}$$

where Γ is the Bromwich contour (i.e. a vertical line in complex plane with its real part to the right of all singularities of the integrand), we obtain (see [12] for further details on the derivation):

$$p(x,t) = \frac{\mathrm{e}^{-\gamma t}}{2} \left\{ \delta\left(x - v_0 t\right) + \delta\left(x + v_0 t\right) + \frac{\gamma}{v_0} \left[I_0(\rho) + \frac{\gamma t I_1(\rho)}{\rho} \right] \Theta\left(v_0 t - |x|\right) \right\}, \tag{1.38}$$

where the paramenter ρ is defined as

$$\rho = \sqrt{v_0^2 t^2 - x^2}\, \frac{\gamma}{v_0} \tag{1.39}$$

and I_0, I_1 are the modified Bessel functions of the first type. They are defined as follows

$$I_n(z) = \frac{1}{\pi} \int_0^\pi e^{z\cos\theta} \cos(n\theta)\, d\theta \quad \text{with } n = 0, 1. \tag{1.40}$$

Chapter 2

A simple model for particles on a line subjected to a resetting dynamics

In this chapter we will retrieve a model already discussed in literature [1] in the case without resetting. We will add a Poissonian resetting rate r at the dynamics and derive analitycally, as far as possible, all the quantities of interest of the system.

2.1 Generalities on the model

To fix ideas we will describe the model in the case of diffusive particles, but the present description is essentially the same also for other dynamics (RTP case is discussed later).
Let us consider a set of N independent particles initially located in the one dimensional domain $[-L, 0] \subset \mathbb{R}$, with $L > 0$ with uniform density $\rho = N/L$ in $[-L, 0]$. Each particle is subjected to a diffusive dynamics with resetting, as already discussed in chapter 1. Let us suppose that the resetting position coincides, for each particle, with its starting position, i.e. indicating with $x_{0,i}$, $X_{r,i}$ respectively the initial and the resetting position of particle i, we have $X_{r,i} = x_{0,i}$ Hence, the Fokker-Planck equation describing the motion of a single particle is

$$\frac{\partial p(x_i, t)}{\partial t} = D\frac{\partial^2 p(x_i, t)}{\partial x^2} - rp(x_i, t) + r\delta(x_i - x_{0,i}) \quad \forall i \tag{2.1}$$

As stated before we consider particles independent, hence we will neglect any type of interaction including excluded-volume one.
The observable we are interested in is Q_t, defined as the flux of particles through the origin up to time t. Each particle crossing the origin from left (right) to right

(left) contributes with $+1(-1)$ to Q_t. It is clear that, as observed in [1], since we start from a step initial condition, this quantity matches with N_t^+, the total number of particles that at time t are found on the positive x-axis. Hence we related a history dependent observable with an instantaneous variable at time t. See figure for a pictorial representation of the situation.

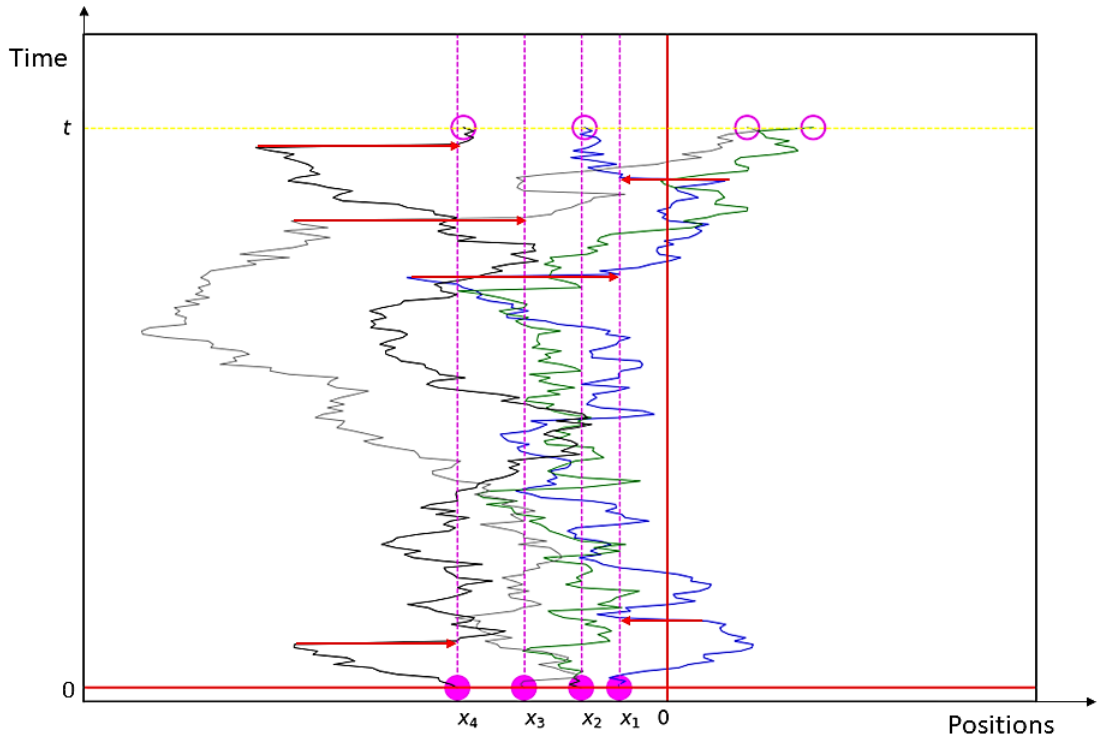

Figure 2.1: The model described above is depicted in the figure. To fix ideas we represented just four particles. Initial positions, indicated with purple filled circles, are denoted with x_1, x_2, x_3, x_4, while final positions are indicated with purple empty circles. Some resetting events are highlighted with red arrows. As we can see, at time t we have two particles on the positive x-axis hence $Q_t = 2$.

We will discuss this model not only for diffusive particles with resetting, but also for RTP with resetting. As we will see, despite the simplicity of the model, a non-trivial dynamical phase transition arises in the case of diffusive particles.

2.1.1 General setting

In this subsection, for the aim of completeness, we will expose the principal relations needed for the description of the system. The treatment follows section 3 of

[1]. For clarity, we will use also the same notation.

Let us recall that we start with a step initial condition where all particles are initialized on the negative x-axis at positions $\{x_1, x_2, \ldots, x_N\}$, where $-L < x_i < 0\ \forall i$. As observed in the previous paragraph, $Q_t = N_t^+$. To compute N_t^+ we could introduce an indicator function $\mathcal{I}_i(t)$ for each particle, such that $\mathcal{I}_i(t) = 1$ if i-th particle is on the positive x-axis at time t, $\mathcal{I}_i(t) = 0$ otherwise. Hence

$$N_t^+ = \sum_{i=1}^{N} \mathcal{I}_i(t). \tag{2.2}$$

For fixed $\{x_i\}$ the flux distribution is given by

$$P\left(Q, t \mid \{x_i\}\right) = \text{Prob}\,.\left(N_t^+ = Q\right) = \left\langle \delta\left[Q - \sum_{i=1}^{N} \mathcal{I}_i(t)\right]\right\rangle_{\{x_i\}} \tag{2.3}$$

where angular brackets $\langle \ldots \rangle_{\{x_i\}}$ denote the average over the history of the system but with fixed initial conditions, we will average later on $\{x_i\}$. Taking the discrete Laplace transform to both sides (i.e. the generating function)

$$\sum_{Q=0}^{\infty} e^{-pQ} P\left(Q, t \mid \{x_i\}\right) = \left\langle e^{-pQ}\right\rangle_{\{x_i\}} = \left\langle \exp\left[-p \sum_{i=1}^{N} \mathcal{I}_i(t)\right]\right\rangle_{\{x_i\}} \tag{2.4}$$

but since the function $\mathcal{I}_i(t)$ can only take values 0 or 1, we can use the identity $e^{-p\mathcal{I}_i} = 1 - (1 - e^{-p})\mathcal{I}_i$ and rewrite

$$\left\langle e^{-pQ}\right\rangle_{\{x_i\}} = \prod_{i=1}^{N} \left[1 - \left(1 - e^{-p}\right) \left\langle \mathcal{I}_i(t)\right\rangle_{\{x_i\}}\right]. \tag{2.5}$$

Since $\mathcal{I}_i(t)$ is an indicator function, its average $\langle \mathcal{I}_i(t)\rangle_{\{x_i\}}$ just gives the probability that i-th particle is found on the positive x-axis at time t given that it started at x_i

$$\left\langle \mathcal{I}_i(t)\right\rangle_{\{x_i\}} = \int_0^{\infty} G\left(x, x_i, t\right) \mathrm{d}x \coloneqq U\left(-x_i, t\right), \quad x_i < 0, \tag{2.6}$$

where we are indicating, as in [1], with $G(x, x_i, t)$ the Green's function, i.e. the propagator for a particle that started at x_i to reach x at time t. Inserting the definition of U we made in (2.6) in equation (2.5) we get

$$\left\langle e^{-pQ}\right\rangle_{\{x_i\}} = \prod_{i=1}^{N} \left[1 - \left(1 - e^{-p}\right) U\left(-x_i, t\right)\right], \quad x_i < 0, \quad \forall i = 1, \ldots, N. \tag{2.7}$$

The validity of the last equation does not rely at all on the specific dynamics of the particles. Indeed, it is valid for any set of non-interacting particles with a common dynamics in one dimension. All informations about the specific dynamics are encoded in the function $U(z,t)$. The idea of our treatment is to invert this Laplace transform and to average over initial positions in order to get $P(Q,t)$. Nevertheless, a special attention is needed for this average which is discussed in the following subsection.

2.1.2 Average over initial positions

As stated before, initial positions are themselves random variables with a certain distribution in the interval $[-L,0]$. As was already observed in [2], in fully analogy to what is done in disordered systems, we could either average over initial positions (as in disordered systems we average the partition function on realizations of the disorder) or consider initial positions fixed and typical (as when we consider partition function for typical values of the disorder). The former case is generally called *annealed average* while the second case goes under the name of *quenched average*. The importance of considering also the quenched case stands in the fact that the typical behavior of the probability could be not captured by the annealed average, since the latter can be dominated by rare realizations of the system.
Therefore, in the following paragraphs we will expose these two cases in detail.

Annealed case We define the annealed distribution $P_{\text{an}}(Q,t)$ through the relation

$$\sum_{Q=0}^{\infty} e^{-pQ} P_{\text{an}}(Q,t) = \overline{\langle e^{-pQ} \rangle_{\{x_i\}}} \tag{2.8}$$

i.e. we are simply averaging equation (2.4) over initial conditions.
Let us compute this average keeping in mind the independence of all particles and the uniform density in the box $[-L,0]$:

$$\overline{\langle e^{-pQ} \rangle_{\{x_i\}}} = \prod_{i=1}^{N} \left[1 - \left(1 - e^{-p}\right) \int_{-L}^{0} U\left(-x_i, t\right) \frac{dx_i}{L} \right] \tag{2.9}$$

$$= \left[1 - \frac{1}{L} \left(1 - e^{-p}\right) \int_{0}^{L} U(z,t) dz \right]^N \tag{2.10}$$

where since the particles are independent we factorized the mean value and since they all undergo the same dynamics the result will be to the power N. Taking the thermodynamical limit, i.e. $L \to \infty$ and $N \to \infty$ but keeping $\rho = N/L$ constant,

we get

$$\sum_{Q=0}^{\infty} e^{-pQ} P_{\text{an}}(Q,t) = \exp\left[-\mu(t)(1-e^{-p})\right], \quad \text{with } \mu(t) = \rho \int_0^{+\infty} U(z,t)\mathrm{d}z. \tag{2.11}$$

If we expand the rhs of (2.11) and compare to the lhs:

$$P_{\text{an}}(Q,t) = e^{-\mu(t)} \frac{(\mu(t))^Q}{Q!} \tag{2.12}$$

i.e., independently from the dynamics, the annealed flux distribution is always a Poissonian distribution with mean $\mu(t)$. The only parameter of the previous formula depending on the specific dynamics of the particles is indeed $\mu(t)$.
We could also analyze the limit for $Q \to +\infty$, $\mu(t) \to +\infty$, keeping $Q/\mu(t)$ fixed. In this case, as found in [1] (simply using Stirling formula), we get

$$P_{\text{an}}(Q,t) \sim \exp\left[-\mu(t)\Psi_{\text{an}}\left(\frac{Q}{\mu(t)}\right)\right] \tag{2.13}$$

with the large deviation function $\Psi_{\text{an}}(q)$ independent of the specific dynamics and of the form

$$\Psi_{\text{an}}(q) = q\ln q - q + 1 \geq 0 \tag{2.14}$$

with the asymptotic behaviors

$$\Psi_{\text{an}}(q) \approx \begin{cases} 1 & \text{as } q \to 0 \\ \frac{1}{2}(q-1)^2 & \text{as } q \to 1 \\ q\ln q & \text{as } q \to \infty \end{cases}. \tag{2.15}$$

$P_{\text{an}}(Q,t)$ shows typical Gaussian fluctuations for Q with mean and variance both equal to $\mu(t)$. In the next sections we will see in detail the calculations to derive all the functions depending on the specific dynamics.

Quenched case The quenched average is defined through the relation

$$\sum_{Q=0}^{\infty} e^{-pQ} P_{\text{qu}}(Q,t) = \exp\left[\overline{\ln\left\langle e^{-pQ}\right\rangle_{\{x_i\}}}\right] \tag{2.16}$$

hence taking the logarithm of equation (2.7)

$$\ln\left[\left\langle e^{-pQ}\right\rangle_{\{x_i\}}\right] = \sum_{i=1}^{N} \ln\left[1 - \left(1-e^{-p}\right) U\left(-x_i,t\right)\right]. \tag{2.17}$$

As before, taking uniform initial conditions in the interval $[-L, 0]$ and letting $N \to \infty$ and $L \to \infty$ but $\rho = N/L$ constant we get

$$\begin{aligned}\overline{\ln\left[\left\langle e^{-pQ}\right\rangle_{\{x_i\}}\right]} &= \frac{N}{L}\int_{-L}^{0} dx_i \ln\left[1-\left(1-e^{-p}\right)U\left(-x_i,t\right)\right] \\ &\to \rho\int_0^{\infty} dz \ln\left[1-\left(1-e^{-p}\right)U(z,t)\right]. \end{aligned} \tag{2.18}$$

Therefore the generating function of quenched flux distribution is

$$\sum_{Q=0}^{+\infty} e^{-pQ} P_{\rm qu}(Q,t) = \exp\left[I(p,t)\right] \tag{2.19}$$

where

$$I(p,t) = \rho\int_0^{+\infty} dz \ln\left[1-\left(1-e^{-p}\right)U(z,t)\right]. \tag{2.20}$$

Unfortunately, at variance with annealed case, this Laplace transform is not simple to invert analytically. Hence, to analyze various regimes, we will consider certain expansions. As usual these expansions are done in [1], here, for the sake of completeness, we report these formulas.

- $p \to 0$ limit: in principle, if we would be able to expand formula (2.20) in powers of p, we could obtain , by comparing the two series term by term, all the momenta of $P_{\rm qu}(Q,t)$. The full analytical expansion is difficult to perform, we will just consider the first two terms of the expansion in order to get the mean and the variance of the flux

  $$I(p,t) = -p\rho\int_0^{\infty} dz\, U(z,t) + \frac{p^2}{2}\rho\int_0^{\infty} dz\, U(z,t)[1-U(z,t)] + \mathcal{O}\left(p^3\right) \tag{2.21}$$

  substituting (2.21) in (2.19), expanding also the exponential in the lhs of (2.19) and comparing term by term:

  $$\langle Q\rangle_{\rm qu} = \rho\int_0^{\infty} U(z,t)dz = \mu(t) \tag{2.22}$$

  $$\sigma^2_{\rm qu} = \left\langle Q^2\right\rangle_{\rm qu} - \langle Q\rangle^2_{\rm qu} = \rho\int_0^{\infty} U(z,t)(1-U(z,t))dz. \tag{2.23}$$

- $p \to +\infty$ limit: in this case we can expand $e^{I(p,t)}$ in powers of e^{-p}. Computing the full expansion, we could obtain the whole function $P_{\rm qu}(Q,t)$, but the expansion is not easy to perform analytically. As before, we could consider just the first two terms to obtain $P_{\rm qu}(Q=0,t)$ and $P_{\rm qu}(Q=1,t)$

  $$I(p,t) = A(t) + B(t)e^{-p} + \mathcal{O}\left(e^{-2p}\right) \tag{2.24}$$

where

$$A(t) = \rho \int_0^\infty \ln[1 - U(z,t)]dz \tag{2.25}$$

$$B(t) = \rho \int_0^\infty \frac{U(z,t)}{1 - U(z,t)}dz, \tag{2.26}$$

substituting this expression and matching the powers of e^{-p} we obtain

$$P_{\text{qu}}(Q = 0, t) = e^{A(t)} = \exp\left[\rho \int_0^\infty \ln\left[1 - U(z,t)\right] dz\right] \tag{2.27}$$

$$P_{\text{qu}}(Q = 1, t) = B(t)e^{A(t)}. \tag{2.28}$$

As usual we stress the fact that all these relations are general, i.e. they depend on the specific dynamics only through the function $U(z,t)$.

2.2 Diffusive dynamics

In this section we will discuss the aforementioned model in the case of a diffusive dynamics with resetting.

2.2.1 Function $U_r(z,t)$

Let us recall from chapter 1 the form of the Green's function Laplace transform (for simplicity we will work in Laplace space):[1]

$$\tilde{G}_r(x, x_i, s) = \frac{1}{\sqrt{4D}} \frac{\sqrt{r+s}}{s} \exp\left(-\sqrt{\frac{r+s}{D}}\ |x - x_i|\right). \tag{2.29}$$

Exploiting the equation (2.6) we can compute the Laplace transform of $U_r(z,t)$

$$\begin{aligned} \tilde{U}_r(z,s) &= \int_0^{+\infty} \frac{1}{\sqrt{4D}} \frac{r+s}{s} \exp\left[-\sqrt{\frac{r+s}{D}}|x+z|\right] \mathrm{d}x \\ &= \frac{1}{2s} \exp\left[-\sqrt{\frac{r+s}{D}}z\right]. \end{aligned} \tag{2.30}$$

This Laplace transform can be inverted exploiting the property of convolution. Indeed, notice that

$$\mathcal{L}^{-1}\left(\frac{1}{2s}\right)(t) = \frac{1}{2}, \tag{2.31}$$

[1] Subscript r indicates resetting case, x_i denotes the initial position.

$$\mathcal{L}^{-1}\left[\exp\left(-\sqrt{\frac{r+s}{D}}z\right)\right](t) = e^{-rt}\mathcal{L}^{-1}\left[\exp\left(-\sqrt{\frac{s}{D}}z\right)\right](t)$$
$$= e^{-rt}\frac{z}{2\sqrt{\pi D t^3}}\exp\left(\frac{z^2}{4Dt}\right), \tag{2.32}$$

where in the intermediate step we used the property of translation, while the latter formula can be taken from tables on Laplace inversions (for instance see [13]). Therefore

$$U_r(z,t) = \int_0^t \frac{z}{4\sqrt{\pi D\tau^3}}\exp\left(-r\tau - \frac{z^2}{4D\tau}\right)\mathrm{d}\tau. \tag{2.33}$$

First of all, we should always check that our result is consistent with the equation $U_0(z,t)$ found in [1], and this is, indeed, the case. Second, we could observe that the limit for t going to $+\infty$ here is clearly dependent on the resetting rate

$$\lim_{t\to+\infty} U_r(z,t) = U_r^{\mathrm{stat}}(z) = \frac{r}{2}\exp\left(-\sqrt{\frac{r}{D}}z\right). \tag{2.34}$$

Nonetheless, the $t \to +\infty$ limit does not provide any information on how the steady state is reached. To analyze this fact we will exploit an idea discussed in [10]. First of all we make the substitution $\tau = ty$, hence the formula rewrites

$$U_r(z,t) = \int_0^1 \frac{zt}{4\sqrt{\pi D t^3 y^3}}\exp\left[-rt\left(y + \frac{1}{4Dry}\left(\frac{z}{t}\right)^2\right)\right]\mathrm{d}y \tag{2.35}$$

$$U_r(z,t) = \int_0^1 \frac{zt}{4\sqrt{\pi D t^3 y^3}}e^{-rt\phi(y,z/t)}\mathrm{d}y \quad \text{with} \quad \phi(y,x) = y + \frac{1}{4Dry}x^2 \tag{2.36}$$

Since we are interested in large time behavior, and since the function ϕ has a unique global minimum, we can approximate the integral with saddle point approximation

$$\frac{\partial}{\partial y}\phi(y,x)\bigg|_{y=y^*} = 0 \quad \Rightarrow \quad 1 - \frac{x^2}{4Dry^{*2}} = 0 \quad \Rightarrow \quad y^* = \sqrt{\frac{x^2}{4Dr}}. \tag{2.37}$$

Where, as could be proven taking the second derivative, y^* corresponds to a minimum.

Hence we must distinguish two cases: when $y^* < 1$ and when $y^* > 1$. In the former case we can evaluate the integral in y^*, while in the latter the minimum of the function ϕ is outside the domain of integration. In this second case, since the function ϕ is strictly decreasing, the integral is dominated by the upper extreme

of integration hence we can evaluate the integral at 1.

$$\text{If } y^* < 1 \Rightarrow U_r(z,t) \sim \exp\left[-rt\left(2\sqrt{\frac{1}{4Dr}}\frac{z}{t}\right)\right] = \exp\left(-\sqrt{\frac{r}{D}}z\right) \tag{2.38}$$

$$\text{If } y^* > 1 \Rightarrow U_r(z,t) \sim \exp\left[-t\left(r + \frac{z^2}{4Dt^2}\right)\right]. \tag{2.39}$$

Where, in the saddle point approximation, the pre-exponential factor does not contribute to the final result. Thus, the function U_r can be written in a large deviation form

$$U_r(z,t) \sim e^{-tf(z/t)}, \quad \text{where} \quad f(u) = \begin{cases} \sqrt{\frac{r}{D}}u & \text{if } u < \sqrt{4Dr} \\ r + \frac{u^2}{4D} & \text{if } u > \sqrt{4Dr} \end{cases}. \tag{2.40}$$

The above expression gives the behavior of $U(z,t)$ in the limit of large t and large z. Interestingly this function f has a discontinuity in the second derivative for $u = u^* = \sqrt{4Dr}$. This hints at the existence of a *dynamical phase transition*. We will see in the next section that a similar discontinuity in the large deviation function can be found also for $P_{\text{qu}}(Q,t)$. An interesting analogy between dynamical phase transitions and equilibrium statistical mechanics is presented in [11]. Essentially, the large deviation function plays the role of a free energy density. Indeed, for extensive systems, for large but finite N, the partition function scales as $Z \sim e^{-\beta N f(\beta)}$ (where β is the inverse temperature and $f(\beta)$ is the free energy density) a formula very similar to (2.40). As a discontinuity in the n-th derivative in the free energy density correspond to a n-th order phase transition of the system, here a discontinuity in one of the derivatives of large deviation function can be seen as a dynamical phase transition for the system.
For what concerns the function $U_r(z,t)$, following a similar argument in [10], a nice interpretation of this kind of phase transition can be given. Essentially, looking at (2.40), there exists an interior spatial region $-\sqrt{4Dr}\ t < z < \sqrt{4Dr}\ t$ where the NESS has been achieved, since no dependence on the time is present anymore, and there is an external region, i.e. $|z| > \sqrt{4Dr}\ t$ in which the NESS has not been estabilished yet. This is pictorially illustrated in the following figure. Therefore, we could say that the phase transition in the function U_r corresponds to a spatial separation between trajectories which reached thermalization and the ones still thermalizing.

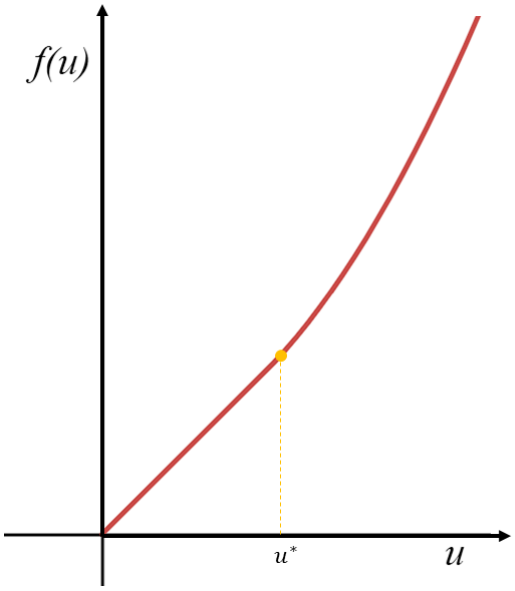

Figure 2.2: The function $f(u)$ is plotted on the left. The point $u^* = \sqrt{4Dr}$ in which there is the discontinuity is highlighted.

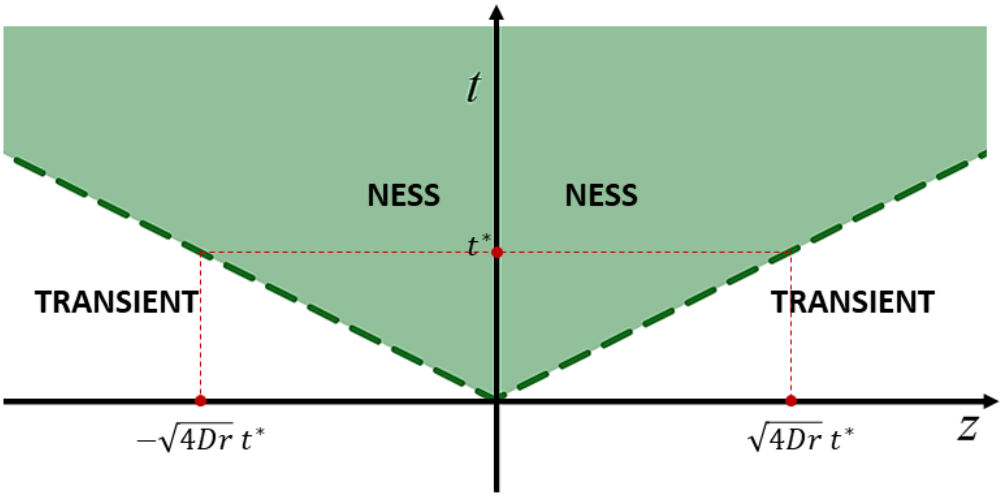

Figure 2.3: Here it is represented the distinction between regions in which the NESS has been estabilished and regions still in a transient. To an arbitrary t^* on time axis, will correspond a region $-\sqrt{4Drt} < z < \sqrt{4Drt}$ on position axis. All particles starting in this region are at thermalization.

2.2.2 Function $\mu_r(t)$

The function $\mu_r(t)$ is defined in (2.11), let us rewrite the definition here

$$\mu_r(t) = \rho \int_0^{+\infty} U_r(z,t)\mathrm{d}z \tag{2.41}$$

Let us compute the integral making use of equation (2.33)

$$\begin{aligned}\mu_r(t) &= \rho \int_0^t \mathrm{d}\tau \frac{e^{-r\tau}}{4\sqrt{\pi D\tau^3}} \int_0^{+\infty} \mathrm{d}z \; z \exp\left(-\frac{z^2}{4D\tau}\right) \\ &= \rho \int_0^t \mathrm{d}\tau \frac{\sqrt{D}e^{-r\tau}}{2\sqrt{\pi\tau}} = \frac{\rho}{2}\sqrt{\frac{D}{r}}\,\mathrm{erf}\left(\sqrt{rt}\right)\end{aligned}$$

$$\mu_r(t) = \frac{\rho}{2}\sqrt{\frac{D}{r}}\,\mathrm{erf}\left(\sqrt{rt}\right) \tag{2.42}$$

Where we inverted the order of integration and we exploited the definition of error function:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\mathrm{d}t$$

As usual, although it is not reported here, in principle we could take the limit for $r \to 0$ and check that this result is consistent to what has been found in [1].

2.2.3 Behaviors in quenched case

As stated before, in the annealed case we are able to compute the exact distribution of P_{an}, while in quenched case this is not analytically possible. Thus, making use of formulas listed in 2.1.2, we will analyze various regimes.

Typical fluctuations: $Q \sim \langle Q \rangle_{\mathrm{qu}}$

$$\langle Q \rangle_{\mathrm{qu}} = \rho \int_0^{\infty} U_r(z,t)dz = \mu(t) = \frac{\rho}{2}\sqrt{\frac{D}{r}}\,\mathrm{erf}\left(\sqrt{rt}\right) \tag{2.43}$$

$$\begin{aligned}\sigma^2_{\mathrm{qu}} = \left\langle Q^2 \right\rangle_{\mathrm{qu}} - \langle Q \rangle^2_{\mathrm{qu}} &= \rho \int_0^{\infty} U_r(z,t)[1 - U_r(z,t)]dz = \\ &= \frac{\rho}{2}\sqrt{\frac{D}{r}}\,\mathrm{erf}\left(\sqrt{rt}\right) - \frac{\rho\sqrt{D}}{8\sqrt{\pi}\sqrt{r}} e^{-2rt} \cdot \\ \cdot \left[\sqrt{\pi} e^{2rt}\left(1 - 2(2rt+1)\,\mathrm{erfc}\left(\sqrt{rt}\right) + (4rt+1)\,\mathrm{erfc}\left(\sqrt{2rt}\right)\right) + 4e^{rt}\sqrt{rt} - 2\sqrt{2rt}\right]\end{aligned} \tag{2.44}$$

Behavior for $Q \gg \langle Q \rangle_{\rm qu}$ The expression of $P_{\rm qu}$ is reported in (2.19). Let us replace the sum with an integral in this formula

$$\int_0^{+\infty} e^{-pQ} P_{\rm qu}(Q,t) dQ = \exp\left[I(p,t)\right]. \tag{2.45}$$

In this paragraph we are interested in finding the large deviation function form of $P_{\rm qu}(Q,t)$, i.e. we want to understand how this function scales in the limit $Q \to +\infty$, $t \to +\infty$ but keeping the ratio Q/t fixed. For reasons that will be clear in the following, this behavior can be analyzed considering the limit $p \to -\infty$ and $t \to +\infty$ with the ratio p/t fixed. For convenience, let us define $v = -p$, then we will take the limit $v \to +\infty$. Recalling the expression of $I(p,t)$ given in (2.20), and the large deviation form of $U_r(z,t)$ given in (2.40), in the large v limit we will have

$$I(-p,t) \coloneqq \tilde{I}(v,t) \approx \rho \int_0^{+\infty} \mathrm{d}z \ln\left[1 + e^{v} e^{-t f(z/t)}\right]. \tag{2.46}$$

To evaluate the integral we make use of the following trick: we first take the partial derivative of the function with respect to v, then we compute the integral and finally we will integrate back in v. The partial derivative reads

$$\begin{aligned} \frac{\partial \tilde{I}(v,t)}{\partial v} &= \rho \int_0^{+\infty} \mathrm{d}z \frac{1}{1 + e^{-[v - t f(z/t)]}} \\ &= \rho t \int_0^{+\infty} \mathrm{d}x \frac{1}{1 + e^{-t[v/t - f(x)]}}. \end{aligned} \tag{2.47}$$

We can recognize that the integral function is a Fermi function and hence for large t, since there is a positive exponential in the denominator, has a step behavior. Thus we can approximate the integral considering just the interval where the function is non-zero. For this reason, let us define x^* as the point such that

$$v - t f(x^*) = 0 \quad \Rightarrow \quad v = t f(x^*)$$

since the function f, formula (2.40), is strictly increasing we have that for $x < x^*$ $f(x) < f(x^*)$ and viceversa. Thus in the region where $x > x^*$ the integrand function is essentially zero, and we can approximate

$$\frac{\partial \tilde{I}(v,t)}{\partial v} \approx \rho t \int_0^{x^*} \mathrm{d}x \frac{1}{1 + e^{-t[f(x^*) - f(x)]}} \approx \rho t x^* = \rho t f^{-1}\left(\frac{v}{t}\right) \tag{2.48}$$

where f^{-1} is the inverse function of f and reads

$$f^{-1}(y) = \begin{cases} \sqrt{\dfrac{D}{r}} y & \text{for } y < 2r \\ \sqrt{4D(y-r)} & \text{for } y > 2r \end{cases} \tag{2.49}$$

Finally integrating back in v

$$\tilde{I}(v,t) = \rho t \int^{v} f^{-1}\left(\frac{y}{t}\right) \mathrm{d}y = \rho t^2 \int^{\frac{v}{t}} f^{-1}(y)\mathrm{d}y = -\rho t^2 \tilde{\phi}\left(\frac{v}{t}\right) \tag{2.50}$$

with

$$\tilde{\phi}(y) = \begin{cases} -\sqrt{\dfrac{D}{r}}\dfrac{y^2}{2} & \text{for } y < 2r \\ -\dfrac{2}{3}\sqrt{Dr^3} - \dfrac{4}{3}\sqrt{Dr^3}\left(\dfrac{y}{r} - 1\right)^{3/2} & \text{for } y > 2r. \end{cases} \tag{2.51}$$

We will make the following ansatz on the large deviation form of $P_{\mathrm{qu}}(Q,t)$

$$P_{\mathrm{qu}}(Q,t) \sim \exp\left[-\rho t^2 \psi\left(\frac{Q}{\rho t}\right)\right] \tag{2.52}$$

thus, substituting in equation (2.45)

$$\begin{aligned} \langle e^{-pQ} \rangle &= \int_0^{+\infty} e^{-pQ} P_{\mathrm{qu}}(Q,t)\mathrm{d}Q \\ &\sim \int_0^{+\infty} \exp\left\{-\rho t^2 \left[\frac{Q}{\rho t^2}p + \psi\left(\frac{Q}{\rho t}\right)\right]\right\} \mathrm{d}Q \end{aligned} \tag{2.53}$$

setting $q = \dfrac{Q}{\rho t}$ and $p = -v$:

$$\langle e^{-pQ} \rangle \sim \int_0^{+\infty} \exp\left\{-\rho t^2 \left[\psi(q) - \frac{v}{t}q\right]\right\} \mathrm{d}q \sim \exp\left[-\rho t^2 \tilde{\phi}\left(\frac{v}{t}\right)\right]. \tag{2.54}$$

Since we are considering the large time behavior we can compute the integral with the saddle point approximation, setting $\dfrac{v}{t} = y$ (recall that the ratio v/t is fixed) and inverting the Legendre transform

$$\min_q \left[\psi(q) - yq\right] = \tilde{\phi}(y) \quad \Rightarrow \quad \psi(q) = \max_y [\tilde{\phi}(y) + qy]. \tag{2.55}$$

Recalling that $\tilde{\phi}$ is a piecewise function, see (2.51), we must distinguish two cases

- For $y < 2r$: $\quad \dfrac{\partial}{\partial y}\left(\tilde{\phi}(y) + qy\right) = \sqrt{\dfrac{D}{r}}y + q \;\Rightarrow\; y^* = \sqrt{\dfrac{r}{D}}q$

$$\Rightarrow \psi(q) = \frac{1}{2}\sqrt{\frac{r}{D}}q^2 \quad \text{for } q < \sqrt{4Dr} \tag{2.56}$$

- For $y > 2r$: $\dfrac{\partial}{\partial y}\left(\tilde{\phi}(y) + qy\right) = -2\sqrt{Dr}\left(\dfrac{y}{r} - 1\right)^{1/2} + q$

  $\Rightarrow y^* = \left(\dfrac{q^2}{4Dr} + 1\right) r$, thus

$$\Rightarrow \psi(q) = -\frac{2}{3}\sqrt{Dr^3} + rq + \frac{q^3}{12D} \quad \text{for } q > \sqrt{4Dr} \tag{2.57}$$

Interestingly, the function ψ has a discontinuity in the third derivative in correspondence of $q^* = \sqrt{4Dr}$, hence the system has a third order phase transition. Notice that for $r = 0$, the phase transition disappears since just one regime is present. Indeed, in [1] authors did not find this phase transition, and thus, the phase transition can be attributed to the presence of resetting. Despite the simplicity of the model, the behavior is rather non-trivial.

For more clarity, let us rewrite all in a more compact form: let us define

$$\psi(q) = \frac{r^2}{\rho}\Psi_{\text{diff}}(q) \quad \Rightarrow \quad P_{\text{qu}}(Q,t) \sim \exp\left\{-r^2t^2\Psi_{\text{diff}}(q)\right\}, \tag{2.58}$$

in the adimensionless variable $q = \dfrac{Q}{rt}$ and with

$$\Psi_{\text{diff}}(q) = \begin{cases} \dfrac{q^2}{q^*} & \text{for } q < q^* = 2\sqrt{\dfrac{D}{r}}\rho \\ -\dfrac{q^*}{3} + q + \dfrac{q^3}{3q^{*2}} & \text{for } q > q^* = 2\sqrt{\dfrac{D}{r}}\rho. \end{cases} \tag{2.59}$$

What we found is an expression of the large deviation form of $P_{\text{qu}}(Q,t)$ valid in the case in which both t and Q tend to $+\infty$ but with the ratio $q = \dfrac{Q}{rt}$ finite. Notice that the first line in (2.59), i.e. when Q is sufficiently smaller than rt, represents stationarity, since substituting in (2.58) time t cancels out. The phase transition founded here arises somehow from the one we founded for the function $U_r(z,t)$ in section 2.2.1. In the last chapter we will see how to simulate the system in order to verify if our analytical calculations are correct.

2.3 Run-and-tumble dynamics

In this section we will discuss the aforementioned model in the case of run-and-tumble dynamics with resetting. We will suppose that each time the particle is reset to its initial position, the velocity is randomized, hence we will have a

probability η that the velocity is the same, and a probability $1-\eta$ that the velocity is reversed after resetting. It was proven by [4, section 6] that, given a symmetric initial condition, the Green function of the process is independent on η, thus we will not care about this parameter η.

2.3.1 Function $U_r(z,t)$

As in the previous part for diffusive particles, here we need the Green's function of the dynamics. We saw in section 1.3.1 the validity of the formula:

$$\tilde{G}_r(x,x_0,s) = \frac{r+s}{s}\ \tilde{G}_0(x,x_0,s), \tag{2.60}$$

this relation relies only on the last renewal property and hence clearly holds also in this case. Therefore, recalling equations (1.36) (1.30), we get

$$\tilde{G}_r(x,x_0,s) = \frac{\lambda(r+s)}{2s}\ e^{-\lambda(r+s)\ |x-x_0|} \tag{2.61}$$

with the function λ

$$\lambda(r+s) = \frac{\sqrt{(r+s)(r+s+2\gamma)}}{v_0}. \tag{2.62}$$

By simply integrating the formula for $\tilde{p}_r$ we can get the expression for $\tilde{U}_r$

$$\tilde{U}_r(z,s) = \frac{r+s}{2s^2} e^{-\lambda(r+s)z}. \tag{2.63}$$

This Laplace transform is not simple to invert, for numerical applications could be useful also the last renewal equation[2] which is reported in the following for completeness

$$U_r(z,t) = e^{-rt}U_0(z,t) + r\int_0^t e^{-r\tau}U_0(z,\tau)d\tau \tag{2.64}$$

where in [1] it has been found the explicit expression of U_0 which is

$$U_0(z,t) = \frac{1}{2}\left[e^{\frac{-\gamma z}{v_0}} + \frac{\gamma z}{v_0}\int_1^{\frac{v_0 t}{z}} dT \frac{e^{\frac{-\gamma z T}{v_0}} I_1\left(\frac{\gamma z}{v_0}\sqrt{T^2-1}\right)}{\sqrt{T^2-1}}\right]\Theta\left(v_0 t - z\right) \tag{2.65}$$

[2]The validity of the last renewal equation also for U_r can be proved by simply integrating the last renewal relation for the Green's function.

2.3.2 Function $\mu_r(t)$

To compute $\mu_r(t)$ we can use the last renewal equation (this relation can be proved by integrating the last renewal equation for U_r)

$$\mu_r(t) = e^{-rt}\mu_0(t) + r\int_0^t e^{-r\tau}\mu_0(\tau)d\tau, \tag{2.66}$$

where the expression of μ_0 has been found in [1]

$$\mu_0(t) = \frac{1}{2}\rho v_0 t e^{-\gamma t}\left[I_0(\gamma t) + I_1(\gamma t)\right] \tag{2.67}$$

where I_0, I_1 are modified Bessel functions of the first kind.

2.3.3 Behaviors in quenched case

Typical fluctuations: $Q \sim \langle Q\rangle_{\text{qu}}$

$$\begin{aligned}\langle Q\rangle_{\text{qu}} &= \mu_r(t) = \\ &= \frac{1}{2}\rho v_0 t e^{-(r+\gamma)t}\left[I_0(\gamma t) + I_1(\gamma t)\right] + \frac{1}{2}\rho v_0 r\int_0^t \tau e^{-(r+\gamma)\tau}\left[I_0(\gamma\tau) + I_1(\gamma\tau)\right]d\tau\end{aligned} \tag{2.68}$$

$$\sigma^2_{\text{qu}} = \left\langle Q^2\right\rangle_{\text{qu}} - \langle Q\rangle^2_{\text{qu}} = \rho\int_0^\infty U_r(z,t)(1 - U_r(z,t))dz \tag{2.69}$$

An analytical expression for these formulas is difficult to obtain, but they can be evaluated numerically.

Behavior for $Q \gg \langle Q\rangle_{\text{qu}}$ The procedure to analyze this behavior is analogous to the one we used in the diffusive case: we replace the sum with an integral

$$\int_0^{+\infty} e^{-pQ}P_{\text{qu}}(Q,t)dQ = \exp[I(p,t)] \tag{2.70}$$

then we try to derivate the large deviation form for $I(p,t)$ in order to substitute this expression in the previous formula. First of all, let us investigate the large deviation form (both z and t large but the ratio z/t finite as usual) for $U_r(z,t)$. Recalling equation (2.63) we can write

$$\tilde{U}_r(z, s-r) = \frac{1}{2(s-r)}\exp\left\{-\sqrt{s(s+2\gamma)}\frac{z}{v_0}\right\}, \tag{2.71}$$

exploiting the saddle point approximation to perform the Laplace inversion, as described also in [1], we can find

$$\mathcal{L}^{-1}\left(\tilde{U}_r(z,s-r)\right)(t) \approx \exp\left\{-\gamma t\left(1-\sqrt{1-\frac{z^2}{v_0^2t^2}}\right)\right\}\Theta(v_0t-z) \tag{2.72}$$

and therefore

$$U_r(z,t) \approx e^{-rt}\exp\left\{-\gamma t\left(1-\sqrt{1-\frac{z^2}{v_0^2t^2}}\right)\right\}\Theta(v_0t-z). \tag{2.73}$$

We are now able to investigate the large deviation form of the quenched distribution, i.e. the regime in which both Q and t are large but the ratio Q/t is finite. As was already explained for diffusive particles, this behavior is found considering the limit for $p \to -\infty$. Thus the computation will be very similar to the previous case. It is convenient to define $u = -p$ in the expression of $I(p,t)$, equation (2.20), and take the limit $u \to +\infty$. For large u we can write

$$I(-p,t) \coloneqq \tilde{I}(u,t) \approx \rho\int_0^{+\infty} \mathrm{d}z \ln\left[1+e^uU_r(z,t)\right]. \tag{2.74}$$

As before, the trick is to take the partial derivative with respect to u, to compute the integral and finally to integrate back in u. The derivative with respect to u reads

$$\frac{\partial\tilde{I}(u,t)}{\partial u} \approx \rho\int_0^{+\infty}\mathrm{d}z\frac{1}{1+\dfrac{e^{-u}}{U_r(z,t)}} \tag{2.75}$$

$$\approx \rho\int_0^{v_0t}\mathrm{d}z\frac{1}{1+\exp\left\{-\left[u-rt-\gamma t\left(1-\sqrt{1-\dfrac{z^2}{v_0^2t^2}}\right)\right]\right\}}. \tag{2.76}$$

We have a Fermi function again. Since we are considering the case in which t is large, the integral will be non-vanishing only when the argument of the exponential is negative. Let us distinguish various regimes:

- $u < rt \Rightarrow$ the integrand function is essentially 0, thus the integral is zero itself. Notice that since we are integrating in the variable z in the interval $[0, v_0t]$, the expression under the square root, i.e. $1-\dfrac{z^2}{v_0^2t^2}$, is always greater than 0 and smaller than 1;

- $rt < u < rt + \gamma t$, in this case there exists a z^* such that the argument of the exponential is 0:

$$z^*(u) \text{ such that } \left[u - rt - \gamma t \left(1 - \sqrt{1 - \frac{z^{*2}}{v_0^2 t^2}} \right) \right] = 0$$

which gives

$$z^*(u) = \frac{v_0}{\gamma} \sqrt{(u - rt)(rt + 2\gamma t - u)}, \tag{2.77}$$

thus for $z < z^*$ the integrand function can be approximated with 1, while for $z > z^*$ the integrand function is essentially 0. We could prove (with very simple algebra) that $z^*(u) \leq v_0 t \ \ \forall u$, hence

$$\frac{\partial \tilde{I}(u,t)}{\partial u} = \rho z^*(u) = \rho \frac{v_0}{\gamma} \sqrt{(u - rt)(rt + 2\gamma t - u)}; \tag{2.78}$$

- $u > rt + \gamma t \Rightarrow$ the argument of the exponential is always negative thus

$$\frac{\partial \tilde{I}(u,t)}{\partial u} \sim \rho v_0 t. \tag{2.79}$$

Integrating back in u to obtain the function $\tilde{I}$ we get

$$\tilde{I}(u,t) = \begin{cases} 0 & u < rt \\ \rho \frac{v_0}{\gamma} \int_{rt}^{u} \sqrt{(x - rt)(rt + 2\gamma t - x)} dx & rt < u < (r + \gamma)t \\ \rho \frac{v_0}{\gamma} \int_{rt}^{rt+\gamma t} \sqrt{(x - rt)(rt + 2\gamma t - x)} dx + \rho v_0 t \left[u - (r + \gamma)t \right] & u > (r + \gamma)t. \end{cases}$$

Thus we can rewrite $\tilde{I}$ in the following large deviation form

$$\tilde{I}(u,t) = \rho \frac{v_0 (r + \gamma)^2}{\gamma} t^2 W \left(\frac{u}{(r + \gamma)t} \right). \tag{2.80}$$

Let us put $y = \dfrac{u}{(r+\gamma)t}$, thus the function $W(y)$ will be

$$W(y) = \begin{cases} 0 & y < \dfrac{r}{r+\gamma} \\ \dfrac{1}{(r+\gamma)^2 t^2} \displaystyle\int_{rt}^{(r+\gamma)ty} \sqrt{(x-rt)(rt+2\gamma t-x)}dx & \dfrac{r}{r+\gamma} < y < 1 \\ \dfrac{1}{(r+\gamma)^2 t^2} \displaystyle\int_{rt}^{(r+\gamma)t} \sqrt{(x-rt)(rt+2\gamma t-x)}dx + \dfrac{\gamma}{r+\gamma}(y-1) & y > 1. \end{cases}$$

Performing the integral we get

$$W(y) = \\ = \begin{cases} 0 & y < 1 - \dfrac{a}{2} \\ \dfrac{1}{4}\sqrt{\left(\dfrac{a}{2}\right)^2 - (1-y)^2}\left[2y - 2 + \dfrac{\sqrt{a^3}\arcsin\left(\sqrt{\dfrac{y-1+a/2}{a}}\right)}{\sqrt{y-1+\dfrac{a}{2}}\sqrt{1-\dfrac{y-1+a/2}{a}}}\right] & 1 - \dfrac{a}{2} < y < 1 \\ \dfrac{1}{16}a^2\pi + \dfrac{a}{2}(y-1) & y > 1 \end{cases} \tag{2.81}$$

where we defined $a = \dfrac{2\gamma}{r+\gamma}$. Notice that the function W has a discontinuity in the second derivative for $y = 1 - \dfrac{a}{2} = y^*$, since

$$\lim_{y\to(y^*)^-} W''(y) = 0, \qquad \lim_{y\to(y^*)^+} W''(y) = +\infty \tag{2.82}$$

and has a discontinuity in the third derivative for $y = 1$. Anyway, as we are going to see, these discontinuities do not lead to phase transitions.
Inserting the large deviation form of $\tilde{I}(u,t)$ in the expression (2.70) and inverting the Laplace transform

$$\begin{aligned} P_{\rm qu}(Q,t) &\approx \int_\Gamma \frac{du}{2\pi i} \exp\left\{-uQ + \rho v_0 \frac{(r+\gamma)^2}{\gamma} t^2\, W\left(\frac{u}{(r+\gamma)t)}\right)\right\} \\ &= \int_\Gamma \frac{du}{2\pi i} \exp\left\{-\rho v_0 \frac{(r+\gamma)^2}{\gamma} t^2 \left(\frac{u}{(r+\gamma)t}\frac{Q}{\rho v_0 \frac{(r+\gamma)t}{\gamma}} - W\left(\frac{u}{(r+\gamma)t}\right)\right)\right\} \\ &\simeq \int_\Gamma \frac{dx}{2\pi i} \exp\left\{-\rho v_0 \frac{(r+\gamma)^2}{\gamma} t^2 \left(x\bar{q} - W(x)\right)\right\} \end{aligned} \tag{2.83}$$

where we set $\bar{q} = \dfrac{Q}{\rho v_0 \dfrac{(r+\gamma)}{\gamma} t}$ and we made the change of variables $x = \dfrac{u}{(r+\gamma)t}$.
Here, as we did for the function U_r, we can exploit saddle point approximation to compute the integral

$$\Psi_{\mathrm{RTP}}(\bar{q}) = \max_x \left[x\bar{q} - W(x)\right]$$
$$\Rightarrow P_{\mathrm{qu}}(Q,t) \sim \exp\left\{-\rho v_0 \frac{(r+\gamma)^2}{\gamma} t^2 \Psi_{\mathrm{RTP}}(\bar{q})\right\} \tag{2.84}$$

The maximum is reached for $x^* = 1 - \dfrac{1}{2}\sqrt{a^2 - 4\bar{q}^2}$, hence x^* is always lower than 1. We could also prove, through simple algebra, that $x^* < 1 - \dfrac{a}{2}$ for any possible choice of the variables, hence discontinuities in the derivatives of W do not influence the dynamics. Therefore, at variance with the diffusive case, here we do not observe the emergence of a dynamical phase transition.
To conclude let us report the full formula for $\Psi_{\mathrm{RTP}}(\bar{q})$

$$\Psi_{\mathrm{RTP}}(\bar{q}) = \bar{q} - \frac{\bar{q}}{4}\sqrt{a^2 - 4\bar{q}^2} - \frac{1}{4}a^2 \arcsin\left(\sqrt{\frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{4\bar{q}^2}{a^2}}}\right) \tag{2.85}$$

with $a = \dfrac{2\gamma}{r+\gamma}$. It can be proved that for $r = 0$ we obtain the expression already found in [1]. It is convenient to rewrite the expression above in the adimensional variable $\alpha = \dfrac{r}{\gamma}$, hence the expressions for a and $\bar{q}$ in function of α are

$$a = \frac{2}{\alpha + 1} \tag{2.86}$$
$$\bar{q} = \frac{1}{\alpha+1}\frac{Q}{\rho v_0 t} = \frac{1}{\alpha+1} q \tag{2.87}$$

where we set $q = \dfrac{Q}{\rho v_0 t}$. Thus we can rewrite the large deviation scaling for $P_{\mathrm{qu}}(Q,t)$ and the corresponding large deviation function as follows

$$P_{\mathrm{qu}}(Q,t) \sim \exp\left\{-\rho v_0 \left(\frac{r}{\gamma} + 1\right) \gamma t^2 \Psi_{\mathrm{RTP}}\left(\frac{Q}{\rho v_0 t}, \frac{r}{\gamma}\right)\right\} \tag{2.88}$$
$$\Psi_{\mathrm{RTP}}(q,\alpha) = q - \frac{1}{\alpha+1}\frac{q}{2}\sqrt{1-q^2} - \frac{1}{\alpha+1}\arcsin\left(\sqrt{\frac{1}{2} - \frac{1}{2}\sqrt{1-q^2}}\right) \tag{2.89}$$

where the only dependence on the resetting rate is in the parameter α. In the regime where $q \ll 1$, i.e. $Q \ll \rho v_0 t$, we can expand the previous equation to get

$$\Psi_{\mathrm{RTP}}(q, \alpha) \simeq \frac{\alpha}{\alpha + 1} q + \frac{1}{6(\alpha + 1)} q^3. \tag{2.90}$$

As explained in chapter 2, for $v_0 \to +\infty$, $\gamma \to +\infty$ but keeping the ratio $\dfrac{v_0^2}{2\gamma} = D_{\mathrm{eff}}$ constant and positive we should retrieve the diffusive case. Indeed, substituting the expansion (2.90) in equations (2.88) (2.89) we get

$$\begin{aligned} P_{\mathrm{qu}}(Q, t) &\sim \exp\left\{ -\rho v_0 (\alpha + 1) \gamma t^2 \left(\frac{\alpha}{\alpha + 1} q + \frac{1}{6(\alpha + 1)} q^3 \right) \right\} \\ &\sim \exp\left\{ \rho v_0 \gamma t^2 \left(\frac{r}{\gamma} \frac{Q}{\rho v_0 t} + \frac{1}{6} \frac{Q^3}{\rho^3 v_0^3 t^3} \right) \right\} \\ &\sim \exp\left\{ -r^2 t^2 \left[\frac{Q}{rt} + \left(\frac{Q}{rt} \right)^3 \frac{r}{12 D_{\mathrm{eff}} \rho^2} \right] \right\} \end{aligned} \tag{2.91}$$

which is, unless a small negative factor, the same expression we found in (2.59). Therefore the matching between the run-and-tumble behavior and the diffusive one can be founded also when a resetting rate is present in the regime $\sqrt{D_{\mathrm{eff}} r}\, \rho t \ll Q \ll \rho v_0 t$.

Chapter 3

Numerical simulations

In this chapter we will see how we can simulate the system in order to check the analytical results found in the previous chapter.

3.1 Diffusive case

3.1.1 Simple sampling

The simplest way to simulate the system is to simply simulate the Langevin equation for each particle, i.e. simulate the stochastic rule (1.2). The computational cost of this operation is extremely high due to the elevated number of steps needed for the convergence of the simulation. Moreover this algorithm is not suitable for importance sampling which is a more sophisticated tecnique used to sample events with very small probabilitities. We will describe importance sampling in the next sections.

A much more efficient way to simulate the system is the following[1]. Keeping in mind the renewal property of all particles, we can describe the state of the particle i through a three-dimensional vector $\vec{v}_i = (x_{0,i}, \tau_i, \Delta x_i)$, where $x_{0,i}$ is the initial position of the particle, τ_i denotes the time elapsed from the last resetting event, and Δx_i denotes the displacement of the particle during this interval τ_i. From the discussions we made in previous sections, $x_{0,i}$ is sampled from a uniform distribution between $[-L, 0]$, τ_i is sampled from an exponential distribution with mean $1/r$ but with the constraint that it cannot exceed the total elapsed time t, and Δx_i is a Gaussian random variable with zero mean and variance $2D\tau_i$. Therefore to simulate the system it is sufficient to sample these three random numbers for each particle. Each particle will contribute to the flux Q with 1 if $x_{0,i} + \Delta x_i > 0$.

[1]The procedure we are going to explain takes inspiration from the algorithm described in [8].

Taking several realizations of the system we can get the histogram of probabilities.

Summarizing, the procedure for annealed case is the following:

1. Observe that the state of the system is enclosed in the $3N$ dimensional vector

$$\vec{V} = (\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_N), \quad \text{with} \quad \vec{v}_i = (x_{0,i}, \tau_i, \Delta x_i) \quad \forall i \tag{3.1}$$

2. Sample the state of each particle:[2]

$$\begin{cases} x_{0,i} \sim \text{Uniform}(-L, 0) & \forall i \\ \tau_i \sim \text{Exp}\left(\dfrac{1}{r}\right) & \forall i \\ \Delta x_i \sim \mathcal{N}(0, 2D\min(\tau_i, t)) & \forall i \end{cases} \tag{3.2}$$

   where the notation $\mathcal{N}(\mu, \sigma^2)$ denotes a Gaussian random number with mean μ and variance σ^2. The third expression comes from the fact that if the system has evolved for a total time t, then the time elapsed from last resetting cannot exceed the value t.

3. Compute the net flux Q considering that

$$\text{if } x_{0,i} + \Delta x_i > 0 \Rightarrow Q \mathrel{+}= 1 \quad \forall i \tag{3.3}$$

   and store this value in a vector $\vec{u}$;

4. Replicate steps $2 \to 4$ for a sufficient number of times. Return vector $\vec{u}$;

5. From $\vec{u}$ construct a probability histogram[3].

The procedure exposed above, since at every step it resamples the initial position, refers to the annealed case. In quenched case, instead, we fix initial positions at the beginning of the algorithm and we update just τ_i and Δx_i. As explained in [1] (but notice that there is a misprint in this paper), a possible choice for $\vec{x}_0$, for the quenched simulation, is the following

$$x_{0,i} = \begin{cases} \sim \text{Uniform}\left(-\dfrac{1}{\rho}, 0\right) & \text{for } i = 1 \\ = x_{0,1} - \dfrac{i-1}{\rho} & \text{for } \; i = 2, \ldots, N \end{cases} \tag{3.4}$$

[2]Notice that it is necessary to follow the order here exposed, since Δx_i depends on the value of τ_i.

[3]The probability histogram is simply constructed by counting the frequencies of the various events.

All the results of the simple sampling algorithm are reported in the figures below. For each of the following simulations we generated 10^7 samples, hence we were just able to investigate probabilities of the order of 10^{-7}. Smaller probabilities can be investigated by means of importance sampling which is described in the next subsection.

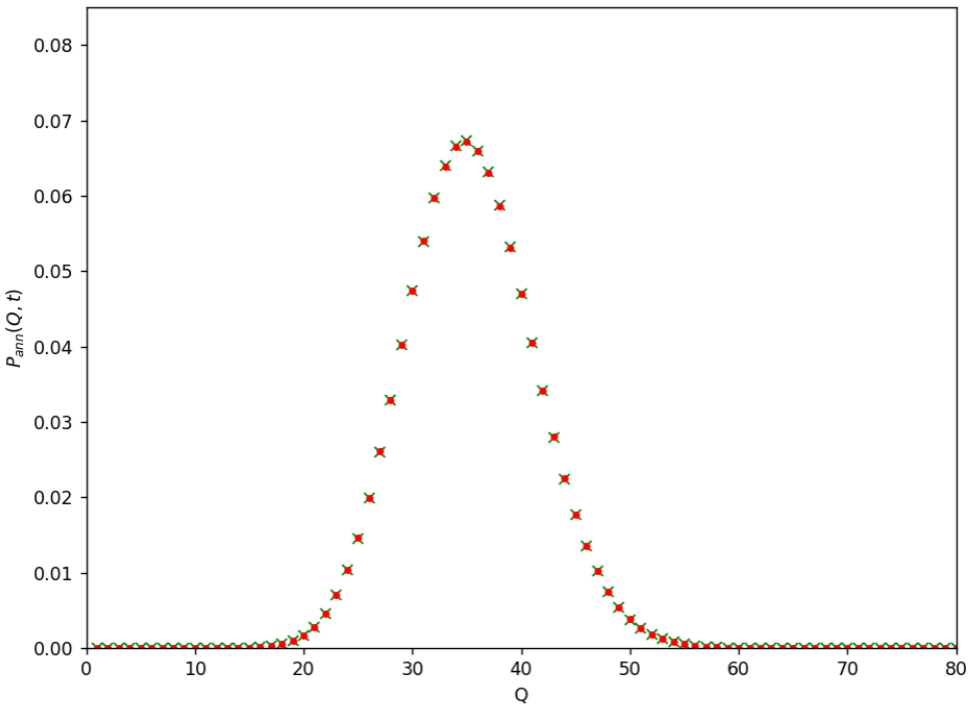

Figure 3.1: Plot of $P_{\text{ann}}(Q,t)$ versus Q. The comparison between simulation and theorical result is shown. Red dots are distributed according to (2.12) with $\mu(t)$ given by (2.42), while the green crosses represent the probabilities resulting from the simulation. The system has been simulated for $N = 10000$, $L = 1000$, $t = 10000$, $r = 0.01$, $D = 0.5$, we averaged over 10^7 samples.

3.1.2 Importance sampling

The algorithm exposed in the previous section, even though it allows us to reconstruct the behavior around typical values, requires a huge amount of time to sample rare events. In this section we will expose an efficient algorithm, based on Markov chain Monte Carlo (MCMC), which allows us to sample arbitrary small probabilities with reasonable short time. In particular we will be able to sample probabilities of the order of 10^{-100}. This tecnique is widely used in stochastic pro-

cesses literature, clearly, it has been used also in [1]. The details of the algorhtm, here exposed in great detail for clarity, can be found in [7] and [9].

As explained in the previous section, the state of the system is enclosed in the vector $\vec{V}$ (formula (3.1)), the idea is to perform a MCMC on $\vec{V}$. We will imagine that each state has a certain Boltzmann weight, we will propose moves on the state vector $\vec{V}$ and we will accept or reject them according to the standard Metropolis rule. To force the system to explore rare trajectories it will be necessary to add a bias to the acceptance rule, but for the moment let us start with the description of the algorithm in the case without bias:

1. Sample a particle, i.e. sample a number in the index set $\{1, \dots, N\}$;

2. Propose a move on the state vector $\vec{v}_i$ of the particle, i.e. transform $\vec{v}_i \to \vec{v}_i^{\text{new}}$, as follows

$$x_{0,i}^{\text{new}} = x_{0,i} + \text{Uniform}(-a, a) \tag{3.5}$$
$$\tau_i^{\text{new}} = \tau_i + \text{Uniform}(-b, b) \tag{3.6}$$
$$\Delta x_i^{\text{new}} = \Delta x_i + \text{Uniform}(-c, c) \tag{3.7}$$

   where a, b, c are positive numbers which are appropriately chosen to make the algorithm converge as fast as possible (generally are heuristically tuned to have a 50% acceptance). As before, this procedure refers to the annealed case, if we are in the quenched case we fix initial position according to the rule (3.4). Let us notice that $x_{0,i}^{\text{new}}$ must be in the interval $[-L, 0]$, hence all moves leading the particle outside this domain are automatically discarded;

3. Accept the move with the Metropolis acceptance rule[4]

$$p_{\text{acc}} = \min\left\{1, \frac{P(\vec{V}^{\text{new}})}{P(\vec{V})}\right\} \tag{3.8}$$

   where $P(\vec{V}^{\text{new}})$ denotes the probability of the proposed state, while $P(\vec{V})$ represents the probability of the old state of the system. Since particles are independent we can factorize

$$P\left(\vec{V}\right) = \prod_{i=1}^{N} p(\vec{v}_i) \tag{3.9}$$

[4]Notice that transition rates cancels. With an abuse of notation, we are indicating with the same letter $p(\dots)$ the probability distribution of whatever random variable. Moreover we use the capital letter for the probability of the state of the whole system $\vec{V}$, while lowercase p refers to the marginal of the state of a single particle.

where $p(\vec{v}_i)$ can be factorized itself

$$p(\vec{v}_i) = p(x_{0,i}, \tau_i, \Delta x_i) = p(x_{0,i})\ p(\tau_i)\ p(\Delta x_i \mid \tau_i) \tag{3.10}$$

and hence, according to (3.2), we have

$$p(\vec{v}_i) = N_0 \frac{1}{L}\ re^{-r\tau_i}\ \exp\left[-\frac{(\Delta x_i)^2}{4D\min(\tau_i, t)}\right], \tag{3.11}$$

where the factor N_0 represents the proper normalization factor, we will not care of N_0 since it cancels in the acceptance probability. Inserting the last equation in (3.8) we get

$$p_{\text{acc}} = \min\left\{1, \exp\left[-\left(\frac{(\Delta x_i^{\text{new}})^2}{4D\min(\tau_i^{\text{new}}, t)} - \frac{(\Delta x_i)^2}{4D\min(\tau_i, t)} + r(\tau_i^{\text{new}} - \tau_i)\right)\right]\right\} \tag{3.12}$$

4. Repeat all the steps $1 \to 4$ until thermalization of the algorithm. When the Markov chain is at thermalization it is possible to take averages of observables. In particular we measured the flux Q every $100N$ steps (each particle did almost 100 steps) in order to avoid correlations in the measure.

5. Construct the histogram of probabilities $P_{\text{an,qu}}(Q, t)$ exploiting the measures did in the previous step.

The algorithm described so far is completely equivalent to the simple sampling. To explore rare realizations of the system — in particular we are interested in estimating the probability of trajectories with $Q \ll \langle Q\rangle$ or $Q \gg \langle Q\rangle$ — we have to introduce a bias in the probability of the state vector $\vec{V}$. The biased probability we considered is the following

$$P_\theta(\vec{V}) = \prod_{i=1}^{N} p_\theta(\vec{v}_i) \tag{3.13}$$

$$\text{with}\ \ p_\theta(\vec{v}_i) = N_\theta \frac{1}{L}\ re^{-r\tau_i}\ \exp\left[-\frac{(\Delta x_i)^2}{4D\min(\tau_i, t)}\right] e^{-\theta Q} \tag{3.14}$$

where N_θ, as before, is a normalization factor while θ is an adjustable parameter called, indeed, bias. It is clear that when $\theta > 0$ configurations with smaller Q are favoured, while $\theta < 0$ pushes the system to explore configurations with $Q > \langle Q\rangle$. Therefore the acceptance probability rewrites

$$p_{\text{acc}} = \min\left\{1, \exp\left[-\left(\frac{(\Delta x_i^{\text{new}})^2}{4D\min(\tau_i^{\text{new}}, t)} - \frac{(\Delta x_i)^2}{4D\min(\tau_i, t)} + \right.\right.\right.$$
$$\left.\left.\left. + r(\tau_i^{\text{new}} - \tau_i) + \theta(Q^{\text{new}} - Q)\right)\right]\right\}. \tag{3.15}$$

Although the acceptance is different, the steps of the algorithm in this case are the same.
Once we have simulated the system with the bias, in order to reconstruct the full shape of the probability histogram, we have to find the correspondence between the unbiased and the biased probabilities. Looking at relations (3.11), (3.14) it is clear that the following equation holds

$$p_\theta(\vec{v}_i) = \frac{N_0}{N_\theta} p_0(\vec{v}_i) e^{-\theta Q} \tag{3.16}$$

and multiplying this relation over all possible indices we have

$$P_\theta(\vec{V}) = \frac{N_0}{N_\theta} P_0(\vec{V}_i) e^{-\theta Q}. \tag{3.17}$$

To find the probability distribution of having a certain value Q we have to integrate the previous equation over all the possible state vectors which leads to $Q_t = Q$, therefore

$$P_{\text{an,qu},\theta}(Q,t) = \frac{N_0}{N_\theta} P_{\text{an,qu}}(Q,t) e^{-\theta Q} \tag{3.18}$$

where the two subscripts mean that the relation is valid in both the annealed and in quenched case. Thus taking the logarithm

$$\log\left[P_{\text{an,qu},\theta}(Q,t)\right] = C_\theta + \log\left[P_{\text{an,qu}}(Q,t)\right] - \theta Q \tag{3.19}$$

where we set

$$C_\theta = \log\left(\frac{N_0}{N_\theta}\right). \tag{3.20}$$

Before *merging* the two histograms, we have to determine the constant C_θ. The procedure to find C_θ is the following: simulate the system for $\theta = 0$ and for $\theta \gtrsim 0$ and construct the two histograms. In the biased simulation we have to choose an appropriate θ in order to have the biased histogram superposing with the unbiased one. In the region where there is the superposition we are able to find the constant C_θ through the formula (3.19). Once we have determined C_θ we can extend the probability histogram using the inverse relation of (3.19):

$$\log\left[P_{\text{an,qu}}(Q,t)\right] = \log\left[P_{\text{an,qu},\theta}(Q,t)\right] - C_\theta + \theta Q \tag{3.21}$$

which allows us to estimate the probability even in regions where the simple sampling gave us null probability.
This procedure can be iterated progressively increasing the bias θ in order to extend further and further the probability histogram. In the following figures some results of importance sampling for annealed distribution are shown.

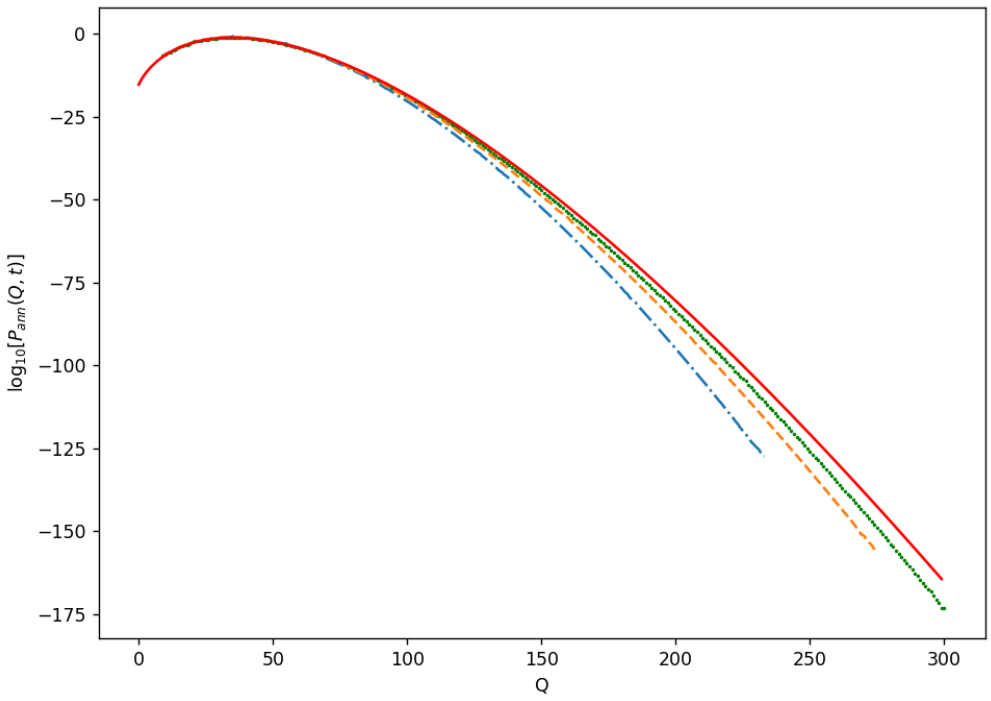

Figure 3.2: Base 10 logarithm of the quenched probability distribution versus Q. The system has been simulated till the bias of $\theta = -4.5$ with the parameters $r = 0.01, D = 0.5, t = 1000, \rho = 10$ for different values of N and L. In particular, the blue line has been obtained with $N = 500, L = 50$, the orange one with $N = 1000, L = 100$, the green one with $N = 2000, L = 200$ while the red curve is the theoretical one given in equation (2.12). As we can see increasing the size of the system the result of the simulation approaches the theoretical result. Moreover, let us notice that importance sampling, in this case, reached probabilities of the order of 10^{-175}. Histograms in this figure have been obtained with $2 \cdot 10^7$ measures of Q.

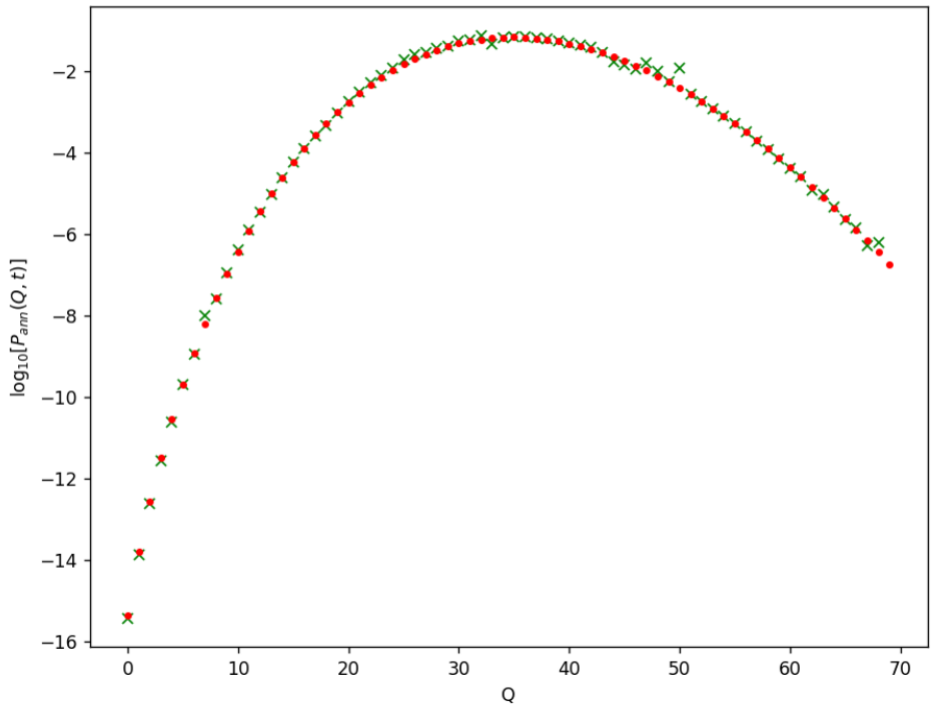

Figure 3.3: Base 10 logarithm of the annealed probability distribution versus Q for small Q. The system has been simulated till the bias of $\theta = 2$ with the parameters $r = 0.01$, $D = 0.5$, $t = 1000$, $N = 2000$, $L = 200$. Red dots represent the theoretical distribution, see equation (2.12), green crosses represent the result of the simulation. The histograms in this figure has been obtained with $2 \cdot 10^7$ measures of Q. As in the previous figure, we can see a quite good agreement with the theoretical result.

Bibliography

[1] Tirthankar Banerjee, Satya N. Majumdar, Alberto Rosso, and Grégory Schehr. Current fluctuations in noninteracting run-and-tumble particles in one dimension. *Phys. Rev. E*, 101:052101, May 2020.

[2] Bernard Derrida and Antoine Gerschenfeld. Current fluctuations in one dimensional diffusive systems with a step initial density profile. *Journal of Statistical Physics*, 137(5-6):978–1000, Sep 2009.

[3] Martin R. Evans and Satya N. Majumdar. Diffusion with stochastic resetting. *Phys. Rev. Lett.*, 106:160601, Apr 2011.

[4] Martin R Evans and Satya N Majumdar. Run and tumble particle under resetting: a renewal approach. *Journal of Physics A: Mathematical and Theoretical*, 51(47):475003, oct 2018.

[5] Martin R Evans, Satya N Majumdar, and Grégory Schehr. Stochastic resetting and applications. *Journal of Physics A: Mathematical and Theoretical*, 53(19):193001, apr 2020.

[6] C. W. Gardiner. *Handbook of stochastic methods for physics, chemistry and the natural sciences*, volume 13 of *Springer Series in Synergetics*. Springer-Verlag, Berlin, third edition, 2004.

[7] Alexander Hartmann, Pierre Doussal, Satya Majumdar, Alberto Rosso, and Gregory Schehr. High-precision simulation of the height distribution for the kpz equation. *EPL (Europhysics Letters)*, 121, 02 2018.

[8] Alexander K Hartmann, Satya N Majumdar, Hendrik Schawe, and Grégory Schehr. The convex hull of the run-and-tumble particle in a plane. *Journal of Statistical Mechanics: Theory and Experiment*, 2020(5):053401, may 2020.

[9] Hartmann, A.K. Large-deviation properties of largest component for random graphs. *Eur. Phys. J. B*, 84(4):627–634, 2011.

[10] Satya N. Majumdar, Sanjib Sabhapandit, and Grégory Schehr. Dynamical transition in the temporal relaxation of stochastic processes under resetting. *Phys. Rev. E*, 91:052131, May 2015.

[11] Satya N. Majumdar and Gregory Schehr. Large deviations, 2017.

[12] P.M.C. Morse and H. Feshbach. *Methods of Theoretical Physics*. International series in pure and applied physics. McGraw-Hill, 1953.

[13] Joel Schiff. *The Laplace Transform: Theory and Applications*. 01 1999.