KU Leuven
Department of Theoretical Physics
Physics Bachelor's Project

Active & Passive Systems in Statistical Mechanics

Current fluctations & large deviations

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Abstract

In this article, a general approach is presented to study the flux distribution through the origin up to a time t, for non-interacting particles with step-initial conditions in one dimension. The focus is on two different cases, diffusive dynamics (passive process) and run-and-tumble-dynamics (active process). We start describing these dynamics using their corresponding stochastic equation of motion, also called the Langevin equation. We then try to find the probability distribution for the position of such a Brownian particle in the case of both dynamics. It will be shown that, for all dynamics, the flux distribution can be described as a Poisson distribution with a mean that only depends on time. This mean will be calculated for both diffusion and run-and-tumble particles (RTP). The particle flux shall be computed and a comparison will be made between the two cases in various limits. We will analyse our results by using numerical simulations and comparing those to our analytical findings.

In dit artikel wordt een algemene methode beschreven voor het bestuderen van de verdeling van de flux door de oorsprong op tijd t, voor niet-interagerende deeltjes met stapsgewijze beginvoorwaarden in één dimensie. De focus ligt hier op twee verschillende gevallen: diffusie (passief proces) en 'run-and-tumble' proces (actief proces). We beschrijven deze dynamische processen door gebruik te maken van de stochastische bewegingsvergelijking, de 'Langevin' vergelijking, die vervolgens gebruikt wordt om de kansverdeling van de positie van een Browniaans deeltje op te stellen. Er zal worden aangetoond dat voor beide gevallen de verdeling van de flux beschreven kan worden door een Poisson verdeling, met een gemiddelde dat enkel van de tijd afhangt. Dit gemiddelde zal berekend worden in het geval van diffusie en het 'run-and-tumble' proces. De flux van de deeltjes zal berekend worden en resultaten voor beide processen zullen in verschillende limieten vergeleken worden. Deze resultaten zullen geanalyseerd worden door gebruik te maken van numerieke simulaties en worden vergeleken met onze analytisch verkregen bevindingen.

Contents

1 Introduction

Real systems encountered in day-to-day life are usually not isolated neither are they in thermodynamic equilibrium. Therefore one usually deals with many-body-problems with a large number of degrees of freedom. In order to describe these degrees of freedom, a 'noise' is introduced and modeled as a random force, otherwise one would require an immense amount of coupled equations to solve such problems. Systems can be pushed out of equilibrium by an external driving force or internal degrees of freedom of the system itself. In this project, the focus is mainly on the second case. Such processes are called active processes in statistical mechanics and many research has been done on this subject.

In this project, two different dynamics will be studied: diffusive dynamics and run-and-tumble dynamics. To understand the system on a microscopic level, the Langevin equation will be used. Run-and-tumble dynamics is executed by E. Coli bacteria. The bacteria will move with a certain speed (run), then randomly change its direction (tumble) in the search for food. The focus is on dynamics in one dimension. Run-and-tumble dynamics is an ideal example of an active process with an internal degree of freedom, the 'tumbling' is the internal degree of freedom due to the fact that it's random and happens with a constant rate of interchange. Here, an overdamped regime is assumed, since the mass of the 'test particle' will be much larger than the particles surrounding this particle.

In order to describe the dynamics, the Langevin equation is used as a starting point. From this, the Fokker-Planck equation will be derived and solved to obtain the probability distribution of the particle's position. The main goal is to describe the flux for non-interacting particles with step-initial conditions. By calculating and comparing the probability of the flux for diffusive and run-and-tumble particles (RTP), the behaviour of the RTP is further studied.

Lastly, some computer simulations can be done using a Monte-Carlo simulation in MATLAB to visualize the dynamics of such Brownian particles. For both dynamics, the path, a certain function $\mu(t)$ (this function will later be specified) and the probability distribution of the flux is plotted. A comparison will be made between the numerical results of the two dynamics and these results will also be compared to our analytical findings.

2 Fokker-Planck equation

The Fokker-Planck equation is a second order partial differential equation describing the time evolution of the probability distribution for Brownian particles. In this section we will derive the Fokker-Planck equation in two distinct cases: diffusion and run-and-tumble. We do this by first giving some heuristic arguments for the particle's probabilistic equation of motion: the Langevin equation. From there we try to find the change in probability of finding a particle at a specific position x at a certain instant in time t. This will ultimaly provide us with the Fokker-Planck equation corresponding to the discussed dynamics.[6]

2.1 Diffusion

Based on [5].

Imagine a particle immersed in a fluid that is at thermal equilibrium at a temperature T. The particle has a mass M and is much larger than the molecules of the fluid. Suppose the particle is moving with a velocity v. Due to the fluid's resistance, the particle will experience a drag force proportional to v, denoted $F_{\text{drag}} = -\gamma v$, where γ is a positive real constant. On the other hand, because of the countless collisions of the particle with the fluid's molecules, the particle will be subject to an immense amount of different forces. All these forces can be well approximated by one random force $f(t)$, called a 'noise'. We assume this noise to have the following properties:

- **Noncorrelation:** The noise $f(t)$ fluctuates at any instant and its value at a time t is independent from that at time t' if $|t - t'| \ggg \tau_0$, where τ_0 is a microscopic time [1].

- **Gaussian distribution:** The noise $f(t)$ is the approximation of all the independent interactions at every instant in time between a large number of fluid-molecules and the test particle of mass M. By the central limit theorem[2], we can conclude the force will be Gaussian distributed.

In the 1 dimensional case, the force distribution is determined by its average and the correlation between two instances in time:

$$\langle f(t) \rangle = 0 \tag{2.1}$$

$$\langle f(t) f(t') \rangle = 2D\gamma^2 \delta(t - t'), \tag{2.2}$$

where D is a constant which will later on be determined as the diffusion coefficient. We call this type of noise 'white noise'. Newton's law of motion then tells us that

$$M \frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + f(t). \tag{2.3}$$

This first order differential equation has a general solution of the form

$$v(t) = v_0 \exp\left[-\frac{\gamma}{M} t\right] + \int_0^t \exp\left[-\frac{\gamma}{M}(t - t')\right] \frac{f(t')}{M} \mathrm{d}t', \tag{2.4}$$

where $v_0 = v(t = 0)$. By taking the average of both sides and remembering (2.1), we get

$$\begin{aligned} \langle v(t) \rangle &= \langle v_0 \rangle \exp\left[-\frac{\gamma}{M} t\right] + \int_0^t \exp\left[-\frac{\gamma}{M}(t - t')\right] \frac{\langle f(t') \rangle}{M} \mathrm{d}t' \\ &= \langle v_0 \rangle \exp\left[-\frac{\gamma}{M} t\right] + 0. \end{aligned} \tag{2.5}$$

[1]The microscopic time τ_0 is given as the duration of a collision between the considered particle and the smaller particles surrounding it.

[2]The central limit theorem states that, when independent random variables are added their sum tends to a normal or Gaussian distribution.

If the diffusive particle were initially to be in equilibrium, $\langle v_0 \rangle$ would be zero. This means that $\forall t \in \mathbb{R}^+ : \langle v(t) \rangle = 0$. Now, as for $\langle v(t)^2 \rangle$, we have to square both sides of equation (2.4) and then take the average. We get

$$\begin{aligned}\langle v(t)^2 \rangle &= \langle v_0^2 \rangle \exp\left[-2\frac{\gamma}{M}t\right] + 2\int_0^t \exp\left[-\frac{\gamma}{M}(t-t')\right] \frac{\langle f(t')v_0 \rangle}{M}\mathrm{d}t' \\ &+ \int_0^t \int_0^t \exp\left[-\frac{\gamma}{M}((t-t_1)+(t-t_2))\right] \frac{\langle f(t_1)f(t_2)\rangle}{M^2}\mathrm{d}t_1\mathrm{d}t_2.\end{aligned}$$

Since $f(t)$ and v_0 are independent, $\langle f(t')v_0 \rangle = 0$, and $f(t)$ obeys (2.2), so this becomes

$$\begin{aligned}\langle v(t)^2 \rangle &= \langle v_0^2 \rangle \exp\left[-2\frac{\gamma}{M}t\right] + \frac{2D\gamma^2}{M^2}\int_0^t \exp\left[-2\frac{\gamma}{M}(t-t')\right]\mathrm{d}t' \\ &= \langle v_0^2 \rangle \exp\left[-2\frac{\gamma}{M}t\right] + \frac{D\gamma}{M}\left(1-\exp\left[-2\frac{\gamma}{M}t\right]\right).\end{aligned}$$

At small timescales, where t is of the order $M/2\gamma$, we see that, when expanding the exponentials and neglecting higher order terms, the second moment of the velocity becomes

$$\begin{aligned}\langle v(t)^2 \rangle &= \langle v_0^2 \rangle \left[1-2\frac{\gamma}{M}t+\dots\right] + \frac{D\gamma}{M}\left[1-1+2\frac{\gamma}{M}t+\dots\right] \\ &= \frac{D\gamma}{M}. \end{aligned} \tag{2.6}$$

This diffusive particle also obeys the equipartition theorem, which states that, in one dimension,

$$\frac{1}{2}M\langle v^2 \rangle = \frac{1}{2}k_B T, \tag{2.7}$$

where k_B is Boltzmann's constant. So, together with (2.6) we find that $D = \dfrac{k_B T}{\gamma}$, which is the diffusion coefficient of the system.

As stated earlier, the Brownian test particle is much larger and much heavier than the particles surrounding it. Therefore we can safely assume the particles motion to be overdamped, meaning $\frac{\mathrm{d}v}{\mathrm{d}t} \approx 0$. The new Langevin equation hence is

$$\dot{x}(t) = v(t) = \frac{f(t)}{\gamma}, \tag{2.8}$$

where the dot denotes the derivative with respect to time. This type of dynamics we will call diffusive dynamics. A particle obeying diffusive dynamics will be called a diffusive particle. Also, this equation has a general solution of the form

$$x(t) = x(0) + \int_0^t \frac{f(t')}{\gamma}\mathrm{d}t'. \tag{2.9}$$

In a time interval Δt, much greater than τ_0, the diffusive particle undergoes a displacement $\Delta x = x(t) - x(0)$ for which

$$\langle \Delta x \rangle = \int_0^t \frac{\langle f(t') \rangle}{\gamma}\mathrm{d}t' = 0 \tag{2.10}$$

and the mean square displacement (MSD) is given by

$$\begin{aligned}\langle \Delta x^2 \rangle &= \frac{1}{\gamma^2}\int_0^t\int_0^t \langle f(t')f(t'')\rangle \mathrm{d}t'\mathrm{d}t'' \\ &= 2D\int_0^t\int_0^t \delta(t'-t'')\mathrm{d}t'\mathrm{d}t'' \\ &= 2D\Delta t. \end{aligned} \tag{2.11}$$

We must mention that (2.11) is dimension-dependent. A diffusive particle in an n-dimensional space has a MSD of $\langle \Delta \mathbf{r}^2 \rangle = 2nD\Delta t$.

Consider now the change of a probability density $P(x,t)$ that a particle following a diffusive trajectory can be found at a position x at time t. The law of total probability states that the probability of an event happening (in this case the particle being at x at time t) can be expressed via the probabilities of several distinct events.[8] Therefore, the probability of finding such a particle at position x at a time $t+\Delta t$ is found by summing al the probabilities of finding a particle at x' at time t, $P(x',t)$, times the probability of that particle being at x at time $t+\Delta t$ given it was at x' at time t, $P(x,t+\Delta t|x',t)$. In mathematical terms

$$P(x,t+\Delta t) = \int P(x',t)P(x,t+\Delta t|x',t)\mathrm{d}x'. \tag{2.12}$$

The distribution of Δx will be denoted by $\phi(\Delta x)$. Using a Taylor series expansion on $P(x',t)$ in powers of Δx around x, we can rewrite (2.12) as

$$P(x,t+\Delta t) = \int \phi(\Delta x)\left[P(x,t) - \Delta x\,\frac{\partial P}{\partial x'}\bigg|_x + \frac{1}{2}\Delta x^2\,\frac{\partial^2 P}{\partial x'^2}\bigg|_x + \dots\right]\mathrm{d}\Delta x,$$

where we did a change in integration variable to Δx. If Δt is small enough, Δx will be small and so we can neglect the higher order terms to find

$$\begin{aligned}
P(x,t+\Delta t) &= P(x,t)\int \phi(\Delta x)\mathrm{d}\Delta x - \frac{\partial P}{\partial x}\int \phi(\Delta x)\Delta x\mathrm{d}\Delta x + \frac{1}{2}\frac{\partial^2 P}{\partial x^2}\int \phi(\Delta x)\Delta x^2\mathrm{d}\Delta x \\
&= P(x,t) - \frac{\partial P}{\partial x}\langle \Delta x\rangle + \frac{1}{2}\langle \Delta x^2\rangle\frac{\partial^2 P}{\partial x^2} \\
&= P(x,t) + \frac{1}{2}(2D\Delta t)\frac{\partial^2 P}{\partial x^2}. \qquad (2.13)
\end{aligned}$$

This means that

$$\frac{P(x,t+\Delta t) - P(x,t)}{\Delta t} = D\frac{\partial^2 P}{\partial x^2}.$$

As $\Delta t \to 0$ this becomes

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}, \tag{2.14}$$

which is the well-known diffusion equation. The solution to this equation is a Gaussian distribution,

$$P(x,x',t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{1}{2}\left(\frac{x'-x}{\sqrt{2Dt}}\right)^2\right], \tag{2.15}$$

with a mean x' and a variance $2Dt$. This probability density can be seen plotted in fig.1 for various values of the mean and variance. Besides (2.15), we can also say that the displacement of a diffusive particle Δx done in a time interval Δt, also has a Gaussian distribution, given as

$$P(\Delta x,\Delta t) = \frac{1}{\sqrt{4\pi D\Delta t}}\exp\left[-\frac{1}{2}\left(\frac{\Delta x}{\sqrt{2D\Delta t}}\right)^2\right], \tag{2.16}$$

with a mean equal to 0 and a variance equal to $2D\Delta t$. This interpretation will be used later on for some numerical simulations in chapter 4.

We can generalize the derivation of (2.14) by including a nonuniform force-field $F(x)$. The Langevin equation then changes to

$$v = \frac{f(t)}{\gamma} + \frac{F(x)}{\gamma}. \tag{2.17}$$

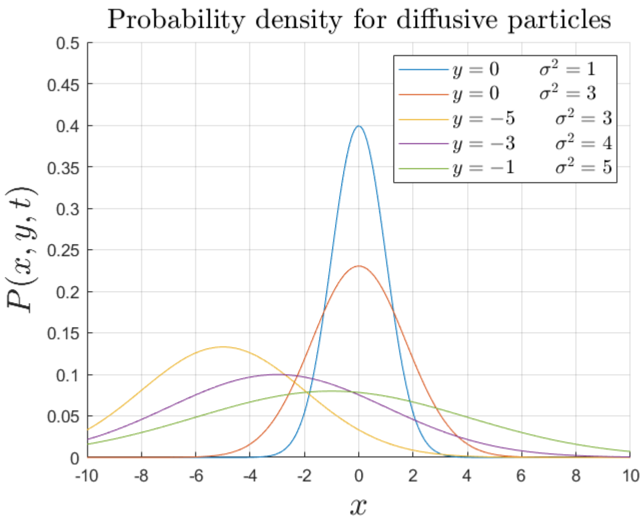


Figure 1: The probability distribution of the position for diffusive particles plotted for different values of the mean y and the variance $\sigma^2 = 2Dt$. We set $D = 0.5$ and used different values for t.

Equation (2.12) can be written as

$$P(x, t + \Delta t) = \int \phi(\Delta x, x')P(x', t)\mathrm{d}x', \tag{2.18}$$

where the distribution ϕ of the displacement Δx now also depends on the initial position x'. To solve for $P(x, t)$ we first introduce an arbitrary function $g(x)$ and try to evaluate its average with respect to $P(x, t + \Delta t)$,

$$\langle g \rangle_{t+\Delta t} = \int g(x)P(x, t + \Delta t)\mathrm{d}x = \int \mathrm{d}x g(x) \int \phi(\Delta x, x')P(x', t)\mathrm{d}x'.$$

By expanding $g(x)$ in Δx around x' and changing the integration variable, $x = x' + \Delta x$, this becomes

$$\langle g \rangle_{t+\Delta t} = \int \int \left[g(x) + \Delta x g'(x) + \frac{1}{2}\Delta x^2 g''(x) + \dots \right] \phi(\Delta x, x')P(x', t)\mathrm{d}x'\mathrm{d}\Delta x. \tag{2.19}$$

In the presence of such a nonuniform force-field, the average of the displacement does not vanish but rather satisfies

$$\langle \Delta x \rangle = \frac{F(x')}{\gamma}\Delta t. \tag{2.20}$$

The MSD is still given by (2.11). Exploiting this and once again neglecting higher order terms, (2.19) becomes

$$\begin{aligned}
\langle g \rangle_{t+\Delta t} &= \int \left[g(x')P(x', t) + g'(x')P(x', t)\langle \Delta x \rangle + \frac{1}{2}g''(x')P(x', t)\langle \Delta x^2 \rangle \right] \mathrm{d}x' \\
&= \int \left[g(x) + \frac{F(x)}{\gamma}\Delta t g'(x) + D\Delta t g''(x) \right] P(x, t)\mathrm{d}x,
\end{aligned}$$

where we changed the integration variable to x. Doing integration by parts, we obtain

$$\begin{aligned}
\langle g \rangle_{t+\Delta t} &= \int g(x)P(x, t)\mathrm{d}x + \int g(x)\Delta t \left[\frac{\partial}{\partial x}\left(-\frac{F(x)}{\gamma}P(x, t) \right) + \frac{\partial^2}{\partial x^2}\left(DP(x, t) \right) \right] \mathrm{d}x \\
&= \langle g \rangle_t + \Delta t \int g(x) \frac{\partial}{\partial x} \left[-\frac{F(x)}{\gamma} + \frac{\partial}{\partial x} D \right] P(x, t)\mathrm{d}x.
\end{aligned}$$

Hence

$$\frac{\langle g\rangle_{t+\Delta t} - \langle g\rangle_t}{\Delta t} = \int g(x)\frac{\partial}{\partial x}\left[-\frac{F(x)}{\gamma} + \frac{\partial}{\partial x}D\right]P(x,t)\mathrm{d}x.$$

If $\Delta t \to 0$, this becomes

$$\frac{\mathrm{d}\langle g\rangle_t}{\mathrm{d}t} = \int g(x)\frac{\partial}{\partial x}\left[-\frac{F(x)}{\gamma} + \frac{\partial}{\partial x}D\right]P(x,t)\mathrm{d}x, \tag{2.21}$$

but we also know that

$$\frac{\mathrm{d}\langle g\rangle_t}{\mathrm{d}t} = \int g(x)\frac{\partial P(x,t)}{\partial t}\mathrm{d}x.$$

Together with (2.21) and the fact that $g(x)$ was an arbitrary function, we ultimately find

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left[-\frac{F(x)}{\gamma} + \frac{\partial}{\partial x}D\right]P. \tag{2.22}$$

This is the Fokker-Planck equation in one dimension and one variable and is also known as the Smoluchowski equation. This is the evolution equation for the probability density.[4] An analytical solution to this equation depends on the nature of the force-field $F(x)$. Since it would take us to far of subject, we will not discuss solutions of (2.22) for various types of force-fields. What we will do is point out that (2.22) can be rewritten in the form of a continuity equation by defining a current $j(x,t)$ as

$$j(x,t) = \left[\frac{F(x)}{\gamma} - \frac{\partial}{\partial x}D\right]P(x,t), \tag{2.23}$$

such that

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x}. \tag{2.24}$$

We discovered that the current is equal to the regular deterministic part, $\dfrac{F(x)}{\gamma}P(x,t)$, and a diffusive part, $D\frac{\partial P(x,t)}{\partial x}$.

2.2 Run-and-Tumble

RTP in one dimension move either to the left or to the right and randomly change direction. We will assume they move with a constant speed v_0 and change direction at an average rate α. The fact that they move to the left or to the right means their velocity is either $-v_0$ or $+v_0$ respectively. We can model this by introducing a function $\sigma(t) = \pm 1$ such that σ switches sign with an average rate α. The switching of $\sigma(t)$ can be seen as an event happening in a certain time interval and is therefore Poisson distributed with average rate α. The noise $v_0\sigma(t)$ is completely characterized by its correlation function at a time delay $\Delta t = t - t'$ which is given by

$$\langle \sigma(t)\sigma(t')\rangle = e^{-2\alpha|t-t'|}. \tag{2.25}$$

This means

$$\langle v(t)v(t')\rangle = \frac{v_0^2}{\alpha}\left[\alpha e^{-2\alpha|t-t'|}\right]. \tag{2.26}$$

If we take the limits $\alpha, v_0 \to \infty$ of (2.26) but keep v_0^2/α fixed, the noise reduces to white noise

$$\langle v(t)v(t')\rangle \to 2D_{\text{eff}}\delta(t-t'), \tag{2.27}$$

where $D_{\text{eff}} := v_0^2/2\alpha$ is the effective diffusion coefficient. We call this the diffusive limit.

Taking in consideration the arguments made earlier, we find that the Langevin equation for RTP can be written as

$$\dot{x} = v_0\sigma(t), \tag{2.28}$$

where the dot denotes the derivative with respect to time. This differential equation has a general solution of the form

$$x(t) = x(0) + \int_0^t v_0\sigma(t')\mathrm{d}t'. \tag{2.29}$$

The MSD, $\langle \Delta x^2 \rangle = \langle [x(t) - x(0)]^2 \rangle$, for RTP can be calculated as follows

$$\begin{aligned}
\langle \Delta x^2 \rangle &= v_0^2 \int_0^t \int_0^t \langle \sigma(t')\sigma(t'') \rangle \mathrm{d}t'\mathrm{d}t'' \\
&= v_0^2 \int_0^t \int_0^t e^{-2\alpha|t'-t''|}\mathrm{d}t'\mathrm{d}t'' \\
&= v_0^2 \int_0^t \left[\int_0^{t''} e^{-2\alpha(t''-t')}\mathrm{d}t' + \int_{t''}^t e^{-2\alpha(t'-t'')}\mathrm{d}t' \right] \mathrm{d}t'' \\
&= v_0^2 \int_0^t \left[\left(\frac{1-e^{-2\alpha t''}}{2\alpha} \right) + \left(\frac{1-e^{-2\alpha(t-t'')}}{2\alpha} \right) \right] \mathrm{d}t'' \\
&= \frac{v_0^2}{2\alpha^2} \left[2\alpha t - 1 + e^{-2\alpha t} \right].
\end{aligned} \tag{2.30}$$

Notice here that, in contrary to the diffusion case, the MSD for RTP is independent of the dimensionality of the space. In the diffusive limit, (2.30) becomes

$$\langle \Delta x^2 \rangle \to 2D_{\text{eff}}\Delta t, \tag{2.31}$$

which is indeed what we'd expect from our result in equation (2.11).

The following derivation is based on [2]

For particles obeying this type dynamics, the probability of finding a particle at position x at time t can be written as

$$P(x,t) = P^+(x,t) + P^-(x,t), \tag{2.32}$$

where $P^\pm(x,t)$ is the probability of finding a particle at position x at time t given $\sigma(t) = \pm 1$. Consider now the probability of finding a particle in position x at a time $t + \mathrm{d}t$ given $\sigma = +1$, denoted by $P^+(x, t + \mathrm{d}t)$. Since particles moving according to (2.28) describe a Markov process[3], this probability is the sum of the probability of a particle being in position $x - \mathrm{d}x$ at time t and $\sigma = +1$ and the probability of a particle being in position $x + \mathrm{d}x$ at time t and $\sigma = -1$. Taking into account the average rate of change of $\sigma(t)$, α, this becomes

$$\begin{aligned}
P^+(x,t+\mathrm{d}t) &= (1-\alpha\mathrm{d}t)P^+(x-\mathrm{d}x,t) + \alpha\mathrm{d}tP^-(x+\mathrm{d}x,t) \\
&= P^+(x-\mathrm{d}x,t) - \alpha\mathrm{d}tP^+(x-\mathrm{d}x,t) + \alpha\mathrm{d}tP^-(x+\mathrm{d}x,t).
\end{aligned}$$

We can expand $P^+(x - \mathrm{d}x, t)$ and $P^-(x + \mathrm{d}x, t)$ in terms of $\mathrm{d}x$ and neglect higher order terms to find

$$\begin{aligned}
P^+(x,t+\mathrm{d}t) &= P^+(x,t) - \frac{\partial P^+(x,t)}{\partial x}\mathrm{d}x - \alpha\mathrm{d}t\left[P^+(x,t) - \frac{\partial P^+(x,t)}{\partial x}\mathrm{d}x\right] + \alpha\mathrm{d}t\left[P^-(x,t) + \frac{\partial P^-(x,t)}{\partial x}\mathrm{d}x\right] \\
&= P^+ - \frac{\partial P^+}{\partial x}\mathrm{d}x - \alpha\mathrm{d}tP^+ + \alpha\mathrm{d}tP^-,
\end{aligned}$$

[3]The position of the particle in the present only depends on the last previous position and not on the entire particle's history.

where $P^{\pm} := P^{\pm}(x,t)$ for convenience. The above can be rewritten as follows

$$\begin{aligned} P^+(x,t+\mathrm{d}t) - P^+(x,t) &= -\frac{\partial P^+}{\partial x}\mathrm{d}x + \alpha \mathrm{d}t\left(P^- - P^+\right) \\ \frac{\partial P^+}{\partial t} &= -\frac{\mathrm{d}x}{\mathrm{d}t}\frac{\partial P^+}{\partial x} + \alpha\left(P^- - P^+\right) \\ &= -v_0\frac{\partial P^+}{\partial x} + \alpha\left(P^- - P^+\right). \end{aligned} \tag{2.33}$$

In an analogous manner we can find that

$$\frac{\partial P^-}{\partial x} = v_0\frac{\partial P^-}{\partial x} + \alpha\left(P^+ - P^-\right), \tag{2.34}$$

and so we are left with a system of two coupled partial differential equations

$$\begin{cases} \partial_t P^+ = -v_0\partial_x P^+ + \alpha\left(P^- - P^+\right) \\ \partial_t P^- = v_0\partial_x P^- - \alpha\left(P^- - P^+\right). \end{cases} \tag{2.35}$$

We can solve these coupled partial differential equations by doing a Laplace transform in t. First remember that, for a function $f(t)$, the Laplace transform of its derivative $f'(t)$ is given by $sF(s) - f(0)$, where $F(s) = \mathcal{L}\{f\}(s)$. This means that the Laplace transform of (2.35) is

$$\begin{cases} s\tilde{P}^+ - P_0^+ = -v_0\partial_x\tilde{P}^+ + \alpha\left(\tilde{P}^- - \tilde{P}^+\right) \\ s\tilde{P}^- - P_0^- = v_0\partial_x\tilde{P}^- - \alpha\left(\tilde{P}^- - \tilde{P}^+\right), \end{cases} \tag{2.36}$$

where we denoted $\tilde{P}^{\pm} := \tilde{P}^{\pm}(x,s) = \mathcal{L}\{P^{\pm}\}(x,s)$ and $P_0^{\pm} = P^{\pm}(x,t=0)$. This system can be written as

$$\begin{cases} 0 = -v_0\partial_x\tilde{P}^+ + \alpha\tilde{P}^- - (s+\alpha)\tilde{P}^+ + P_0^+ \\ 0 = v_0\partial_x\tilde{P}^- + \alpha\tilde{P}^+ - (s+\alpha)\tilde{P}^- + P_0^-, \end{cases} \tag{2.37}$$

or, in matrix form

$$\frac{\mathrm{d}}{\mathrm{d}x}\begin{pmatrix}\tilde{P}^+ \\ \tilde{P}^-\end{pmatrix} = \underbrace{\begin{pmatrix} -\dfrac{s+\alpha}{v_0} & \dfrac{\alpha}{v_0} \\ -\dfrac{\alpha}{v_0} & \dfrac{s+\alpha}{v_0} \end{pmatrix}}_{:=A}\begin{pmatrix}\tilde{P}^+ \\ \tilde{P}^-\end{pmatrix} + \begin{pmatrix}P_0^+ \\ P_0^-\end{pmatrix}. \tag{2.38}$$

If we fix these initial conditions such that the particle starts at position y and the probabilities are symmetric, we have

$$P_0^+ = P_0^- = \frac{1}{2}\delta(x-y). \tag{2.39}$$

We can solve (2.38) away from the initial position y. Since A is a constant matrix we can use the eigenvalue method to solve this system of differential equations. The eigenvalues λ of A obey

$$\det(A - \lambda\mathbb{I}) = 0,$$

so

$$\lambda(s) = \pm\left[\frac{s(s+2\alpha)}{v_0^2}\right]^{\frac{1}{2}} \tag{2.40}$$

Hence, the solution is of the form

$$\begin{pmatrix}\tilde{P}^+ \\ \tilde{P}^-\end{pmatrix} = \mathbf{v}_1 e^{\lambda(x-y)} + \mathbf{v}_2 e^{-\lambda(x-y)}, \quad \text{where } \mathbf{v}_1 = \begin{pmatrix}v_{11} \\ v_{12}\end{pmatrix} \text{ and } \mathbf{v}_2 = \begin{pmatrix}v_{21} \\ v_{22}\end{pmatrix}. \tag{2.41}$$

$\tilde{P}^{\pm}$ must be finite as $x \to \pm\infty$ so

$$\begin{pmatrix} \tilde{P}^+ \\ \tilde{P}^- \end{pmatrix} = \mathbf{v}_2 e^{-\lambda(x-y)} \quad \text{if } x > y \qquad \text{and} \qquad \begin{pmatrix} \tilde{P}^+ \\ \tilde{P}^- \end{pmatrix} = \mathbf{v}_1 e^{\lambda(x-y)} \quad \text{if } x \leq y$$

This means $\tilde{P}(x,s)$ is given by

$$\tilde{P}(x,s) = \begin{cases} v_{11}e^{\lambda(x-y)} + v_{12}e^{\lambda(x-y)} & \text{when } x \leq y \\ v_{21}e^{-\lambda(x-y)} + v_{22}e^{-\lambda(x-y)} & \text{when } x > y. \end{cases} \tag{2.42}$$

Next, since the initial conditions are symmetric about the origin and the dynamics are invariant under time reversal, the probability should be symmetric about the origin. This means

$$\begin{aligned} \tilde{P}^+(x \leq y, s) + \tilde{P}^-(x \leq y, s) &= \tilde{P}^+(x > y, s) + \tilde{P}^-(x > y, s) \\ v_{11}e^{\lambda(x-y)} + v_{12}e^{\lambda(x-y)} &= v_{21}e^{-\lambda(x-y)} + v_{22}e^{-\lambda(x-y)}. \end{aligned}$$

As $x \to y$, we find

$$v_{11} + v_{12} = v_{21} + v_{22}. \tag{2.43}$$

What we also know is that the integral of $P(x,t)$ over $-\infty < x < \infty$ is equal to 1. Hence

$$\begin{aligned} \int_0^\infty \int_{-\infty}^\infty e^{-st} P(x,t)\mathrm{d}x\mathrm{d}t &= \int_0^\infty e^{-st}\mathrm{d}t \\ \int_{-\infty}^\infty \tilde{P}(x,s)\mathrm{d}x &= \frac{1}{s}. \end{aligned}$$

And so, if we keep in mind $\tilde{P}(x,s)$ is given by (2.42),

$$\begin{aligned} \int_{-\infty}^\infty \tilde{P}(x,s)\mathrm{d}x &= \int_{-\infty}^y \left[v_{11}e^{\lambda(x-y)} + v_{12}e^{\lambda(x-y)} \right] \mathrm{d}x + \int_y^\infty \left[v_{21}e^{-\lambda(x-y)} + v_{22}e^{-\lambda(x-y)} \right] \mathrm{d}x \\ &= \frac{v_{11}+v_{12}}{\lambda} + \frac{v_{21}+v_{22}}{\lambda} = \frac{1}{s} \end{aligned} \tag{2.44}$$

By using both (2.43) and (2.44), we ultimately find that

$$v_{11} + v_{12} = v_{21} + v_{22} = \frac{\lambda}{2s}. \tag{2.45}$$

This means that

$$\tilde{P}(x,s) = \begin{cases} \dfrac{\lambda}{2s} e^{\lambda(x-y)} & \text{if } x \leq y \\ \dfrac{\lambda}{2s} e^{-\lambda(x-y)} & \text{if } x > y, \end{cases} \tag{2.46}$$

or just

$$\tilde{P}(x,s) = \frac{\lambda(s)}{2s} e^{-\lambda(s)|x-y|} \quad \text{where } \lambda(s) = \frac{\sqrt{s(s+2\alpha)}}{v_0}. \tag{2.47}$$

This is the Laplace transform in time of the probability distribution for the position of RTP. We could try to perform an inverse Laplace transform to obtain $P(x,t)$ but this is unnecessary if we only want to know the particle flux of this dynamics. The reason for this will become clear in section 3.3.

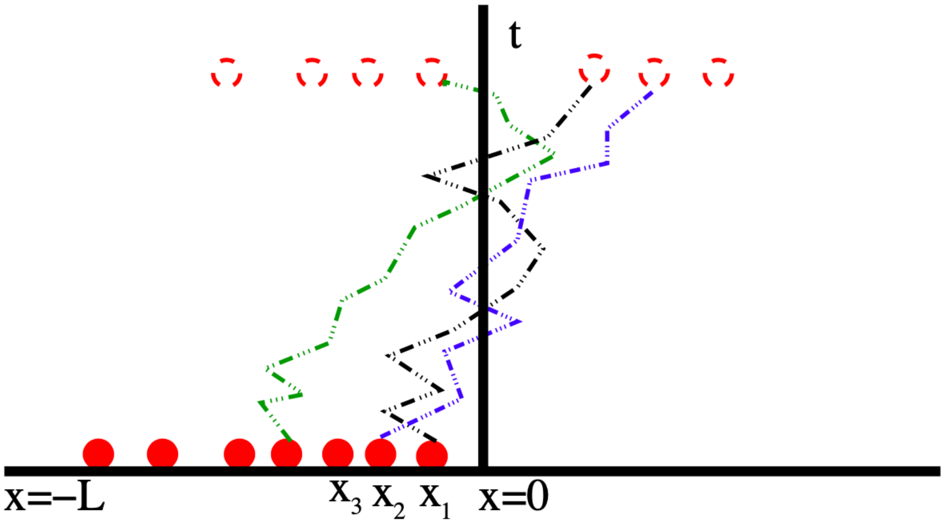


Figure 2: N particles uniformly distributed across the interval $[-L, 0]$ on the x-axis and their random movements in time. [1]

3 Particle Flux

3.1 General Setting

Consider a set of N particles uniformly distributed along the interval $[-L, 0]$ on the x-axis as shown in figure 2. At time $t = 0$ the particle density is $\rho = N/L$. Label the particles $i = 1, 2, \dots, N$ and denote the position of the i-th particle at time t as $x_i(t)$. The position of these particles evolve depending on the type of dynamics the system follows. Our goal is to find an expression for the particle flux $Q(t)$ past the origin up to a certain instant in time t. A particle crossing from the negative side of the x-axis to the positive side contributes $+1$ to the net particle current. Each particle crossing in the opposite direction contributes -1. The total flux Q is the total contribution to the net particle current up to time t. This means that the flux Q up to time t is the number of particles at the right side of the y-axis at time t, denoted as $N^+(t)$. We can introduce an indicator function $I_j(t)$ such that

$$I_j(t) = \begin{cases} 1 & \text{if} \quad x_j(t) > 0 \\ 0 & \text{if} \quad x_j(t) < 0, \end{cases} \quad \text{with } j = 1, 2, \dots, N.$$

The number of particles on the positive side of the x-axis is then given by

$$N^+(t) = \sum_{j=1}^{N} I_j(t).$$

For a fixed set of initial conditions $\{x_i\}$ the probability of finding a flux Q at time t is given by

$$P(Q, t, \{x_i\}) = \text{Prob.}(N^+(t) = Q) = \left\langle \delta \left[Q - \sum_{j=1}^{N} I_j(t) \right] \right\rangle_{\{x_i\}},$$

where $\langle \dots \rangle_{\{x_i\}}$ denotes the average over the history given a certain set of initial conditions $\{x_i\}$. To find an expression for the probability distribution of the flux Q at a time t we start by doing a Laplace transform in Q.

$$
\begin{aligned}
\tilde{P}(\nu,t,\{x_i\}) = \sum_{Q=0}^{N} e^{-\nu Q} P(Q,t,\{x_i\}) &= \left\langle \sum_{Q=0}^{N} e^{-\nu Q} \delta\left[Q - \sum_{j=1}^{N} I_j(t)\right] \right\rangle_{\{x_i\}} \\
&= \left\langle \exp\left[-\nu \sum_{j=1}^{N} I_j(t)\right] \right\rangle_{\{x_i\}} \\
&= \prod_{j=1}^{N} \left\langle \exp\left[-\nu I_j(t)\right] \right\rangle_{\{x_i\}}
\end{aligned} \tag{3.1}
$$

Since $I_j(t)$ can only take the values 0 or 1 we can write the exponential as

$$
e^{-\nu I_j(t)} = 1 - \left(1 - e^{-\nu}\right) I_j(t) \quad \text{where } j = 1, 2, \ldots, N. \tag{3.2}
$$

Substituting (3.2) in (3.1) gives

$$
\tilde{P}(\nu,t,\{x_i\}) = \prod_{j=1}^{N} \left[1 - \left(1 - e^{-\nu}\right) \langle I_j(t)\rangle_{\{x_i\}}\right]. \tag{3.3}
$$

We assume the particles are non-interacting. This means

$$
\tilde{P}(\nu,t,\{x_i\}) = \left[1 - \left(1 - e^{-\nu}\right) \langle I_j(t)\rangle_{\{x_i\}}\right]^N. \tag{3.4}
$$

Writing this as the exponential of a natural logarithm gives

$$
\tilde{P}(\nu,t,\{x_i\}) = \exp\left\{N \ln\left[1 - (1 - e^{-\nu})\langle I_j(t)\rangle_{\{x_i\}}\right]\right\}. \tag{3.5}
$$

By taking the average over all initial conditions, denoted as $\overline{P(Q,t,\{x_i\})} := P_a(Q,t)$, the Laplace transform becomes

$$
\begin{aligned}
\tilde{P}_a(\nu,t) &= \sum_{Q=0}^{N} e^{-\nu Q} \overline{P(Q,t,\{x_i\})} \\
&= \sum_{Q=0}^{N} e^{-\nu Q} P_a(Q,t) \\
&= \exp\left\{N \ln\left[1 - (1 - e^{-\nu})\overline{\langle I_j(t)\rangle}\right]\right\},
\end{aligned} \tag{3.6}
$$

where $\overline{\langle I_j(t)\rangle}$ is given by

$$
\begin{aligned}
\overline{\langle I_j(t)\rangle} &= \int_0^\infty \overline{P(x,x_j,t)} \mathrm{d}x \\
&= \int_0^\infty \int_{-L}^{0} P(x,x_j,t) \frac{\mathrm{d}x_j}{L} \mathrm{d}x
\end{aligned} \tag{3.7}
$$

and $P(x,x_j,t)$ is the probability of finding a particle at position x at time t given it started at position x_j. This probability distribution of the position of a particle depends entirely on the type of dynamics the particle obeys. By using (3.7) in (3.6) and doing a Taylor expansion of the natural logarithm in $(1 - e^{-\nu})\overline{\langle I_j(t)\rangle}$ up until first order we get

$$
\tilde{P}_a(\nu,t) = \exp\left[-\frac{N}{L}(1 - e^{-\nu}) \int_0^\infty \int_{-L}^{0} P(x,x_j,t) \mathrm{d}x_j \mathrm{d}x\right]. \tag{3.8}
$$

When taking the limits $N \to \infty$, $L \to \infty$ but keeping $\rho = N/L$ fixed and doing a change of variables $x_j = -y$ this becomes

$$\tilde{P}_a(\nu, t) = \exp\left[-\rho(1-e^{-\nu})\int_0^\infty \int_0^\infty P(x, -y, t)\mathrm{d}y\mathrm{d}x\right]. \tag{3.9}$$

The double integral can be rewritten as just a function of the time t. Let's define this function as

$$\mu(t) := \rho \int_0^\infty \int_0^\infty P(x, -y, t)\mathrm{d}x\mathrm{d}y \tag{3.10}$$

This function will be crucial in determining the probability distribution of the flux. It also solely depends on the dynamics of the particle. The Laplace transform of the probability distribution of the flux is then given by

$$\sum_{Q=0}^{\infty} e^{-\nu Q} P_a(Q, t) = \exp\left[-\mu(t)(1-e^{\nu})\right]. \tag{3.11}$$

This expression can be recognized as being the moment generation function of a Poisson distribution $M(-\nu) = \mathrm{E}\left[e^{-\nu Q}\right]$ but the probability distribution of the flux can also be derived explicitly by doing an inverse Laplace transform. Using the Bromwich integral (based on [7]) to find the inverse Laplace transform $f(t) = \mathcal{L}^{-1}\{F(s)\}(t)$ of a Laplace transformed function $F(s)$, which is defined as,

$$f(t) = \frac{1}{2\pi i}\int_{\gamma-\infty}^{\gamma+i\infty} e^{st}F(s)\mathrm{d}s \tag{3.12}$$

gives,

$$P_a(Q, t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{\nu Q}\exp\left[-\mu(t)(1-e^{\nu})\right]\mathrm{d}\nu. \tag{3.13}$$

Here, γ is a vertical line such that $\mathrm{Re}(\gamma)$ is greater than all the real parts of the singularities of $\exp\left[-\mu(t)(1-e^{\nu})\right]$. Since this expression has no poles, we can take $\gamma = 0$ which means we can also do a convenient change of variables and set $\nu = ik$. This results in

$$P_a(Q, t) = \frac{e^{-\mu(t)}}{2\pi i}\int_{-\infty}^{\infty} e^{ikQ}\exp\left[\mu(t)e^{ik}\right] i\mathrm{d}k. \tag{3.14}$$

We can write one of the exponentials in the integrand as a power series expansion

$$\begin{aligned} P_a(Q, t) &= \frac{e^{-\mu(t)}}{2\pi}\int_{-\infty}^{\infty} e^{ikQ}\left[\sum_{n=0}^{\infty}\mu(t)^n\frac{e^{-ikn}}{n!}\right]\mathrm{d}k \\ &= e^{-\mu(t)}\sum_{n=0}^{\infty}\frac{\mu(t)^n}{n!}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(Q-n)}\mathrm{d}k\right], \end{aligned} \tag{3.15}$$

where the term inside the straight brackets is an expression for the Dirac delta function which is 1 when $Q = n$ and 0 otherwise. Hence

$$\begin{aligned} P_a(Q, t) &= e^{-\mu(t)}\sum_{n=0}^{\infty}\frac{\mu(t)^n}{n!}\delta(Q-n) \\ &= e^{-\mu(t)}\frac{\mu(t)^Q}{Q!} \quad \text{with } Q \in \mathbb{N}. \end{aligned} \tag{3.16}$$

Finally, we see that $P_a(Q, t)$ is indeed a Poisson distribution with both mean and variance equal to $\mu(t)$. This is the case for any type of dynamics. Also, finding the probability distribution $P_a(Q, t)$ of the particle flux across the origin for different types of dynamics is reduced to obtaining the function $\mu(t)$ as defined by (3.10) for each type of dynamics. Notice that the probability of having a zero flux up to time t is given by

$$P_a(Q=0,t) = e^{-\mu(t)}, \tag{3.17}$$

which drops of to zero for non-biased random dynamics[4] quickly as time increases. Since all the particles started from the negative side of the x-axis, the flux at time $t = 0$ is 0 and so $P_a(Q = 0, t = 0) = 1$. This means that $\lim_{t\to 0} \mu(t) = 0$ for all types of dynamics. Also notice that equation (3.16) can be rewritten according to

$$\begin{aligned} P_a(Q,t) &= \exp\left[\ln\left(e^{-\mu(t)}\frac{\mu(t)^Q}{Q!}\right)\right] \\ &= \exp\left[-\mu(t) + \ln\left(\frac{\mu(t)^Q}{Q!}\right)\right] \\ &= \exp\left[-\mu + \ln\left(\mu(t)^Q\right) - \ln(Q!)\right]. \end{aligned}$$

When taking the limits $Q \to \infty$ and $\mu(t) \to \infty$ but keeping $Q/\mu(t)$ fixed, we can use Stirling's approximation formula for the factorial, giving

$$\begin{aligned} P_a(Q,t) &\approx \exp\left[-\mu(t) + Q\ln\mu(t) - Q\ln Q + Q\right] \\ &= \exp\left[-\mu(t) + Q\ln\left(\frac{\mu(t)}{Q}\right) + Q\right] \\ &= \exp\left[-\mu(t)\psi(q)\right], \end{aligned} \tag{3.18}$$

where we defined $q := Q/\mu(t)$ and

$$\psi(q) := q\ln q - q + 1. \tag{3.19}$$

This is the large deviation function and is plotted in figure 3. We see that

$$\psi(q) = \begin{cases} 1 & \text{as } q \to 0 \\ \dfrac{(q-1)^2}{2} & \text{as } q \to 1 \\ q\ln q & \text{as } q \to \infty. \end{cases} \tag{3.20}$$

The quadratic behaviour of ψ as q approaches 1 points out typical Gaussian fluctuation of Q with both mean and variance equal to $\mu(t)$. The dependence on the dynamics in (3.18) only comes from $\mu(t)$, $\psi(q)$ is independent of the dynamics.

3.2 Diffusive dynamics

As previously discussed in section 2.1 the probability distribution of finding a diffusive particle at a position x at time t, given it started from a position y is given by a Gaussian function

$$P(x,y,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\left(\frac{x-y}{\sqrt{4Dt}}\right)^2\right], \tag{3.21}$$

which means that $\mu(t)$ in the case of diffusive dynamics is

$$\mu(t) = \rho\int_0^\infty\int_0^\infty \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\left(\frac{x+y}{\sqrt{4Dt}}\right)^2\right]\mathrm{d}x\mathrm{d}y. \tag{3.22}$$

[4]Random dynamics which include a force-field are biased in the sense that this force-field ‘pushes’ the Brownian particles in a certain direction.

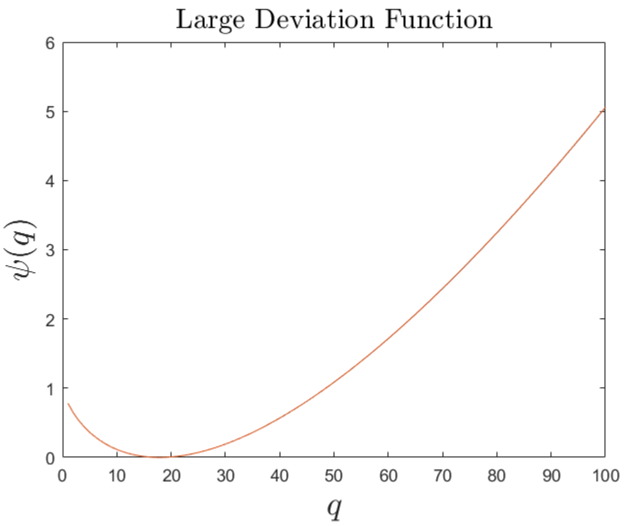


Figure 3: The large deviation function for both diffusive particles and RTP after a time $t = 1000$ and diffusion coefficients $D = D_{\text{eff}} = 1$.

This is a double integral of a Gaussian function which is not a straightforward calculation. To evaluate this double integral and eventually find $\mu(t)$ we first consider

$$\int_0^\infty \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\left(\frac{x+y}{\sqrt{4Dt}}\right)^2\right] \mathrm{d}x = \int_{y/\sqrt{4Dt}}^\infty \frac{1}{\sqrt{\pi}} e^{-z^2} \mathrm{d}z, \tag{3.23}$$

where y is considered a constant for now and we did a change in variables by setting $z = \dfrac{x+y}{\sqrt{4Dt}}$. This new integral is known as the complementary error function which is given by

$$\begin{aligned} \operatorname{erfc}(a) = 1 - \operatorname{erf}(a) &= 1 - \frac{1}{\sqrt{\pi}} \int_{-a}^{a} e^{-t^2} \mathrm{d}t \\ &= \frac{2}{\sqrt{\pi}} \int_a^\infty e^{-t^2} \mathrm{d}t. \end{aligned}$$

This means that

$$\int_0^\infty \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\left(\frac{x+y}{\sqrt{4Dt}}\right)^2\right] \mathrm{d}x = \frac{1}{2} \operatorname{erfc}\left(\frac{y}{\sqrt{4Dt}}\right).$$

Using this, we find that (3.22) is equivalent to

$$\mu(t) = \rho \int_0^\infty \frac{1}{2} \operatorname{erfc}\left(\frac{y}{\sqrt{4Dt}}\right) \mathrm{d}y. \tag{3.24}$$

Another change in variables brings us to

$$\mu(t) = \rho \frac{\sqrt{4Dt}}{2} \int_0^\infty \operatorname{erfc}(s) \mathrm{d}s. \tag{3.25}$$

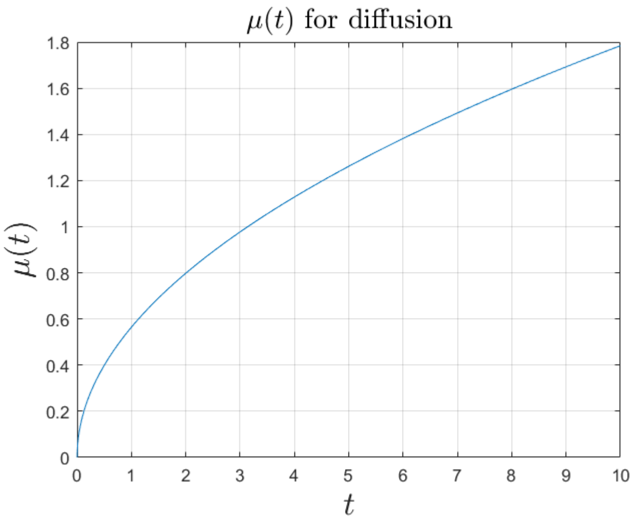


Figure 4: A plot of $\mu(t)$ in the case of diffusion with a diffusion coefficient $D = 1$ and an initial particle density $\rho = 1$.

If we note that $\frac{\mathrm{d}}{\mathrm{d}a}\mathrm{erfc}(a) = \frac{\mathrm{d}}{\mathrm{d}a}\left[1 - \mathrm{erf}(a)\right] = \frac{\mathrm{d}}{\mathrm{d}a}\left[1 - \frac{2}{\sqrt{\pi}}\int_0^a e^{-t^2}\mathrm{d}t\right] = -\frac{2}{\sqrt{\pi}}e^{-a^2}$ we can do integration by parts to find

$$\begin{aligned}
\mu(t) &= \rho\sqrt{Dt}\left[s \cdot \mathrm{erfc}(s)|_0^\infty - \int_0^\infty s\frac{\mathrm{d}}{\mathrm{d}s}\mathrm{erfc}(s)\mathrm{d}s\right] \\
&= \rho\sqrt{Dt}\left[0 + \frac{2}{\sqrt{\pi}}\int_0^\infty se^{-s^2}\mathrm{d}s\right] \\
&= \rho\sqrt{\frac{Dt}{\pi}}.
\end{aligned} \tag{3.26}$$

We've finally established that, in the case of diffusion, $\mu(t) = \rho\sqrt{Dt/\pi}$ and this can be seen plotted in fig. 4. The probability distribution for the flux of diffusive particles is thus given by

$$P_a(Q,t) = \exp\left[-\rho\sqrt{\frac{Dt}{\pi}}\right]\frac{\left(\rho^2\frac{Dt}{\pi}\right)^{\frac{Q}{2}}}{Q!} \qquad \text{with } Q \in \mathbb{N}. \tag{3.27}$$

3.3 Run-and-tumble dynamics

Based on [3]

From (2.47) we can say that a particle, which started at a position y has a "Laplace transformed probability" of being in position x at transformation variable s given by

$$\tilde{P}(x,y,s) = \frac{\lambda(s)}{2s}e^{-\lambda(s)|x-y|}. \tag{3.28}$$

Using (3.10) and the inverse Laplace transform, we can write

$$\mu(t) = \rho\int_0^\infty\int_0^\infty\left[\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}e^{st}\tilde{P}(x,-y,s)\mathrm{d}s\right]\mathrm{d}x\mathrm{d}y, \tag{3.29}$$

where, once again, γ is a vertical line such that $\mathrm{Re}(\gamma)$ is greater than the real part of the singularities of $\tilde{P}(x,-y,s)$. Rewriting this gives

$$\begin{aligned}\mu(t) &= \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{st}\left[\rho\int_0^\infty\int_0^\infty \tilde{P}(x,-y,s)\mathrm{d}x\mathrm{d}y\right]\mathrm{d}s \\ &= \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{st}\tilde{\mu}(s)\mathrm{d}s, \end{aligned} \tag{3.30}$$

where we defined $\tilde{\mu}(s)$ as

$$\tilde{\mu}(s) := \rho\int_0^\infty\int_0^\infty \tilde{P}(x,-y,s)\mathrm{d}x\mathrm{d}y. \tag{3.31}$$

We can evaluate $\tilde{\mu}(s)$ by using (3.28) to find

$$\tilde{\mu}(s) = \rho\int_0^\infty\int_0^\infty \frac{\lambda(s)}{2s}e^{-\lambda(s)|x+y|}\mathrm{d}x\mathrm{d}y, \tag{3.32}$$

where $\lambda(s)$ is still given by (2.40). Since we integrate x and y over the positive real axis, this becomes

$$\begin{aligned}\tilde{\mu}(s) &= \frac{\rho\lambda(s)}{2s}\int_0^\infty\int_0^\infty e^{-\lambda(s)(x+y)}\mathrm{d}x\mathrm{d}y \\ &= \frac{\rho\lambda(s)}{2s}\int_0^\infty e^{-\lambda(s)x}\left[\int_0^\infty e^{-\lambda(s)y}\mathrm{d}y\right]\mathrm{d}x \\ &= \frac{\rho}{2s\lambda(s)}. \end{aligned} \tag{3.33}$$

To eventually find $\mu(t)$ for run-and-tumble dynamics, we have to do an inverse Laplace transform of (3.33). We do this by using 'Mathematica'[5] and find

$$\mu(t) = \frac{\rho v_0}{2}te^{-\alpha t}\left[I_0(\alpha t) + I_1(\alpha t)\right], \tag{3.34}$$

where I_n are the modified Bessel functions of the first kind given by

$$I_n(x) = \sum_{m=0}^{\infty}\frac{1}{m!\Gamma(m+n+1)}\left(\frac{x}{2}\right)^{2m+n} \tag{3.35}$$

and α is still the average rate of change of $\sigma(t)$. We have plotted the first two modified Bessel functions and their sum in fig. 5a for $\alpha = 0.5$ and we notice that these have the form of exponentials. Also $\mu(t)$ for the RTP case is plotted in figure 5b. Here we see that $\mu(t)$ in the run-and-tumble case has the same form as $\mu(t)$ in the diffusion case as seen in figure 4. These similarities will be further discussed in chapter 4.

The behaviour of $\mu(t)$ for RTP in the case of $t \to 0$ can be found by neglecting higher-order term of the modified Bessel functions. We find that

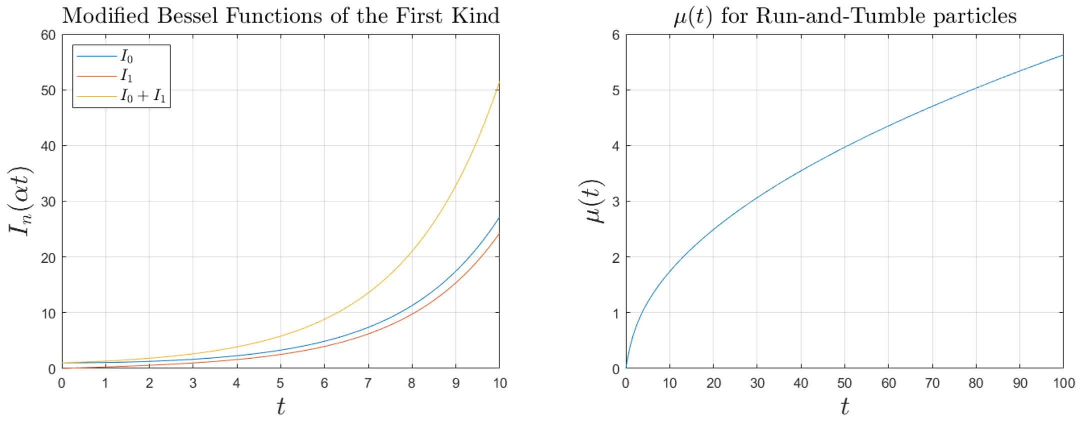
$$\mu(t) = \frac{\rho v_0}{2}t \qquad \text{as } t \to 0. \tag{3.36}$$

From figure 5b we can make an educated guess that

$$\mu(t) = \sqrt{\frac{D_{\mathrm{eff}}t}{\pi}} \qquad \text{as } t \to \infty, \tag{3.37}$$

where D_{eff} is once again the effective diffusion coefficient. This guess implicates that RTP behave as diffusive particles in the large time regime.

[5] Note that for the inverse Laplace transform given in (3.13) we did not use Mathematica since we had to explicitly show that the flux Q could indeed only take discrete values.



(a) (b)

Figure 5: **Left:** Plots of the modified Bessel functions of the first kind, I_0 and I_1, and their sum with a value $\alpha = 0.5$. **Right:** Plot of the function $\mu(t)$ for RTP with the values $\alpha = 0.5$; $v_0 = 1$ and $\rho = 1$.

By substituting (3.34) (or (3.36) and (3.37) in the proper limits) into (3.16) we find the probability distribution for the particle flux in the case of RTP.

We must also note that, from (2.28), the maximum distance an RTP can travel in a time t is $\Delta x_{\max} = v_0 t$. This means that the maximum flux after a time t, in the case of RTP, is given by the number of particles at a distance smaller than $v_0 t$ from the origin. Since we have a uniform particle density ρ, the maximum flux is given by $Q_{\max} = \rho v_0 t$. The probability distribution in time, for $Q = Q_{\max}$ is plotted in figure 6. Here we see that the probability of having the maximum possible amount of flux drastically drops to zero when $t > 0$.

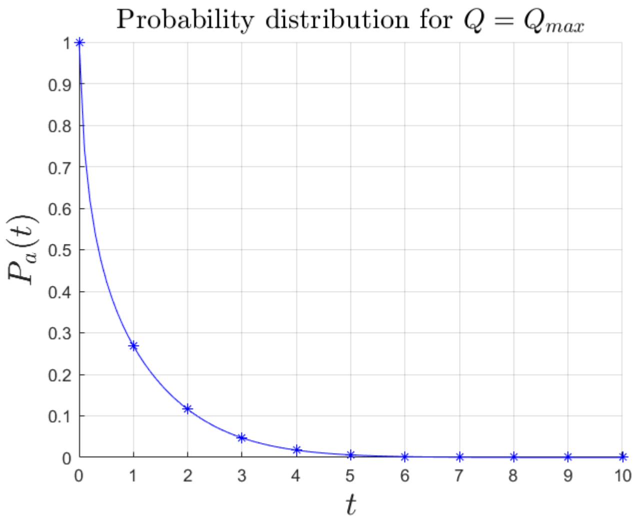


Figure 6: The probability distribution of having the maximum possible amount of particle flux, with a particle density $\rho = 1$, a velocity $v_0 = 1$ and an average rate of switching $\alpha = 0.5$. The points indicated by an asterisk are the different values of $Q_{\max}$ in the corresponding time. The value on the horizontal axis is, in this case, also the maximum flux, while the value on the vertical axis is the probability of having such a flux at time t.

4 Numerical simulations

In this chapter we will use Monte Carlo simulations in MATLAB to obtain some numerical results on the paths taken by the Brownian particles, the function $\mu(t)$ and the probability distributions of the flux in time for diffusion as well as for RTP. These numerical results will then be compared to our analytical findings. We will use arbitrary units for all our quantities.

4.1 Random Paths

Once again we denote the position of the i-th particle at time t as $x_i(t)$, where $i = 1, 2, \ldots, N$. We found the displacement Δx of a diffusive particle done in a time interval Δt to be Gaussian distributed. This Gaussian distribution has a vanishing mean and a variance $2D\Delta t$ as was shown in (2.16). From this, we can deduce:

$$\Delta x_i = \sqrt{2D\Delta t}X \tag{4.1}$$

where $i = 1, 2, \ldots, N$ and X is an arbitrary stochastic variable such that $X \sim \mathcal{N}(0, 1)$. Hence

$$x_i(t + \Delta t) = x_i(t) + \sqrt{2D\Delta t}X. \tag{4.2}$$

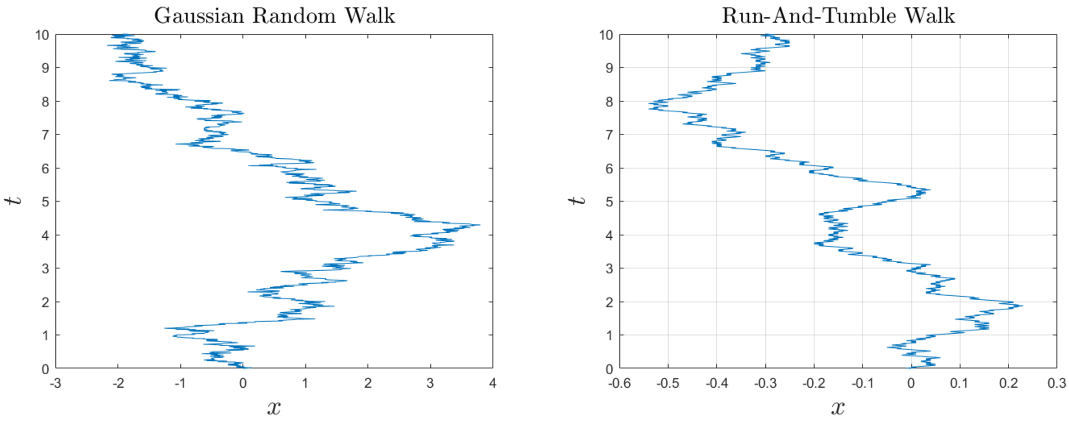
A random walk of this nature is called a Gaussian random walk. Let's look at a single diffusive particle starting from the origin, meaning $x(0) = 0$. Take the diffusion coefficient to be $D = 1$ and the time interval during which the particle undergoes a displacement Δx to be $\Delta t = 0.01$. A particle moving like this, taking 1000 steps, follows a path that looks like the one in figure 7a.

As for RTP, the dynamics is given by (2.28) and so we can write down an similar equation to (4.2) in an analogous manner, namely

$$x_i(t + \Delta t) = x_i(t) + v_0\sigma(t)\Delta t. \tag{4.3}$$

Consider once again a single particle now obeying (2.28). Take, for example, $\alpha = 0.5$ and $v_0 = 1$, meaning the effective diffusion coefficient is $D_{\text{eff}} = 1$. The switching of $\sigma(t)$ is Poisson distributed and so the probability of σ having changed sign after an interval Δt is given as

$$P(\sigma \text{ switches an odd amount of times}) = \sum_{k=0}^{\infty} \frac{(\alpha\Delta t)^{2k+1}}{(2k+1)!} e^{-\alpha\Delta t}, \tag{4.4}$$



(a) (b)

Figure 7: Note that, although the position x of the Brownian particle is a function of time t, we've plotted x on the horizontal axis and t on the vertical axis. This way the plots are in better agreement with the initial conditions proposed in fig.2. **Left:** The path of a single particle performing a Gaussian random walk with a diffusion coefficient $D = 1$. **Right:** The path of a single particle performing run-and-tumble motion with an average rate of change $\alpha = 0.5$ and a standard velocity $v_0 = 1$. These paths are entirely stochastic so every numerical simulation of such a path will be different.

since α is the average rate of change of σ. Now, as Δt becomes really small, we can approximate this probability by neglecting higher-order terms

$$P(\sigma \text{ switches an odd amount of times}) \approx [\alpha\Delta t + \dots]\left[1 - \alpha\Delta t + \frac{(\alpha\Delta t)^2}{2} + \dots\right] \tag{4.5}$$

$$\approx \alpha\Delta t[1 - \alpha\Delta t]. \tag{4.6}$$

We can simulate the random change in sign of σ by taking a random standard normal distributed variable and checking whether it is smaller than the value given by (4.6) or not. If the random variable is smaller, σ switches sign. A particle taking 1000 step according to (4.3) follows a path which looks like the one plotted in figure 7b.

4.2 The function $\mu(t)$

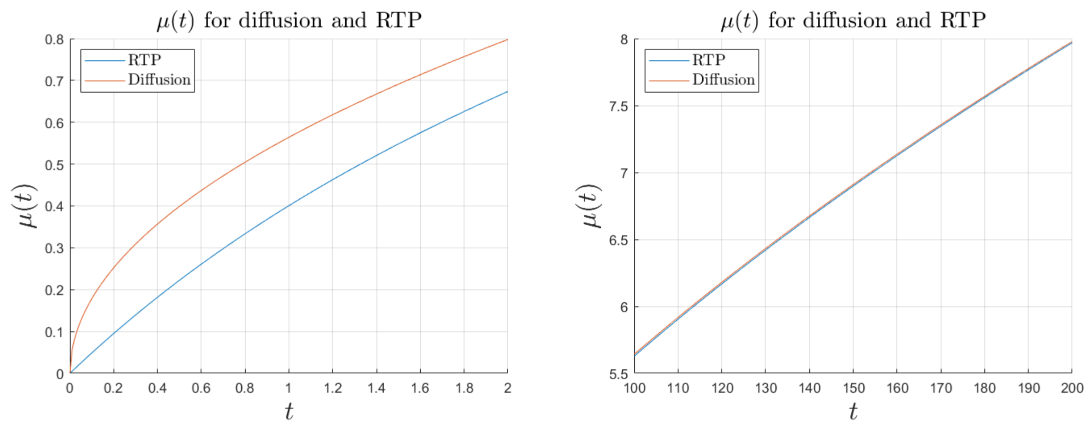
As was showed in chapters 3.2 and 3.3, the function $\mu(t)$ for diffusion and RTP is given as

$$\mu_{\text{diff}}(t) = \rho\sqrt{\frac{Dt}{\pi}} \tag{4.7}$$

$$\mu_{\text{RTP}}(t) = \frac{\rho v_0}{2} t e^{-\alpha t}[I_0(\alpha t) + I_1(\alpha t)], \tag{4.8}$$

respectively. We saw these two plotted in figures 4 and 5b and we can compare these in the case of $D = D_{\text{eff}}$ in the small and large time regimes as is shown in figure 8a and 8b respectively. We see that, in the small time regime, there is a relatively large discrepancy between $\mu_{\text{diff}}(t)$ and $\mu_{\text{RTP}}(t)$. The diffusion case increases very quickly around $t = 0$, thereafter the increase appears to slow down, while the RTP case seems to have a more linear behaviour right from $t = 0$ throughout the small time regime.

In the large time regime, we see that $\mu_{\text{diff}}(t)$ and $\mu_{\text{RTP}}(t)$ practically coincide. This means our educated guess, made in (3.37), is now numerically justified and RTP flux does indeed behave as if it were diffusion in the large time regime with an effective diffusion coefficient $D_{\text{eff}} = v_0^2/2\alpha$.



(a) (b)

Figure 8: Plots of $\mu_{\text{diff}}(t)$ (in orange) and $\mu_{\text{RTP}}(t)$ (in blue) with $D = D_{\text{eff}} = 1$ in the small time regime (**left**) and the large time regime (**right**).

4.3 Probability Distributions

In this section we will explain and perform the numerical 'experiments' with which we will try to confirm our analytical results concerning the probability distributions of the flux for both the diffusion and RTP case. We will obtain numerical outcomes regarding the probability distribution $P_a(Q,t)$ vs. Q at different times and $P_a(Q,t)$ vs. t for different amount of fluxes.

4.3.1 Diffusion

Consider 100 particles uniformly distributed along the horizontal axis on the interval $[-100, 0]$, such that the particle density ρ is just 1, as was discussed in section 3.1. Each of these particles will perform a Gaussian random walk with a diffusion coefficient $D = 1$ and we inspect the diffusive particle flux after a time $t = 1000$. This flux is given by the number of particles on the right-hand side of the origin. Finally the particles are reset to the initial conditions and the same process is repeated.[6] This is done 1000 times. The flux can be different each of these 1000 times. The received data can be seen represented in fig. 9. From this we see that the average of the flux, which is at the maximum of the curve, at a time $t = 1000$ is approximately 17. From our analytical results, using (3.26), we'd find an average flux by evaluating $\mu_{\text{diff}}(t = 1000) \approx 17.84$. Notice that only a certain range in flux values is obtained. All the other flux values have a numerical probability of 0.

By fitting the relative amounts[7] of each flux value together with the analytical predicted Poisson distribution given by (3.27) we can check if the Monte Carlo simulations reproduce the analytical results. We still use the same numerical values as stated above. This fitting is done in figure9. We see that the data received from the Monte Carlo simulations matches decently (especially around the mean) with the analytically predicted curve.

[6]Note that the initial conditions of the particles are different each time. The positions are chosen randomly from a uniform distribution.

[7]Meaning the total number of times a certain flux is obtain divided by the amount of time the experiment is conducted.

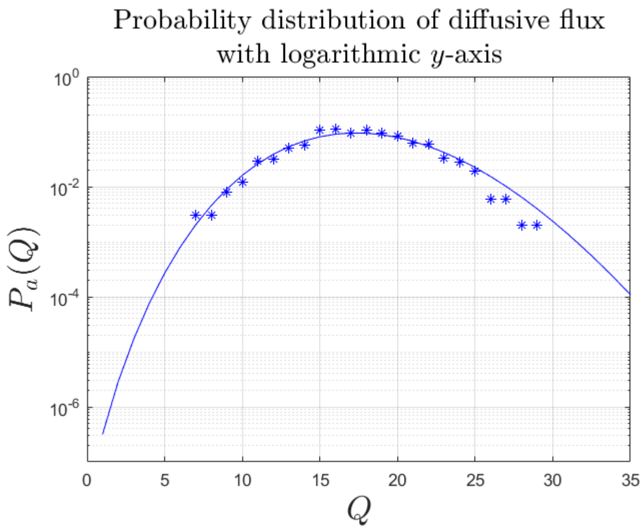


Figure 9: A semi-log plot of the probability distribution $P_a(Q,t)$ vs. the flux Q up to a time $t = 1000$ for diffusive particles. The diffusion coefficient is $D = 1$. The blue asterisks indicate the different flux values and their corresponding probabilities as obtained by the Monte Carlo simulations. The solid blue line is the analytical predicted distribution.

We can plot this probability distribution function for different times. These will always have the form of a Poisson distribution as can be seen in figure 10a. It can be seen clearly that the curve flattens as time increases. The peak broadens with time. This is due to the fact that, for diffusive particles, the variance on the position also increases with time.

Another possibility is to see how the probability distribution varies in time for different flux values[8]. We can see from (3.27) that the peak of the distribution for a fixed flux $Q = n$ will be at

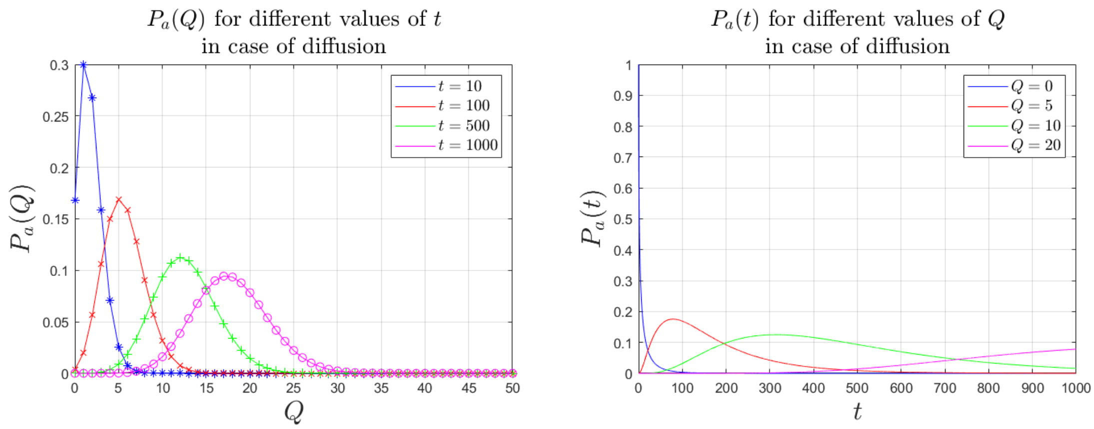
$$t = \left(\frac{n}{\rho}\right)^2 \frac{\pi}{D}.$$

The probability at this peak will be

$$P_a\left(t = \left(\frac{n}{\rho}\right)^2 \frac{\pi}{D}\right) = e^{-n}\frac{n^n}{n!}$$

and we see that this peak shifts to the right and flattens as n increases. Also the probability of having zero flux is, ofcourse, 1 at $t = 0$ but then drastically drops off to a near zero probability. It is thus a very unlikely event to find a zero flux at times $t > 0$.

[8]With this we mean to examine the possibility of having a flux $Q = n$ throughout time.



(a) (b)

Figure 10: In both pictures we consider the diffusion case with a diffusion coefficient $D = 1$. **Left:** Plots of the probability distribution $P_a(Q,t)$ vs. the flux Q at different times. The different possible flux values between 0 and 50 are marked and their corresponding probability is read from the vertical axis. **Right:** Probability distribution $P_a(Q,t)$ vs time t for different small flux values Q.

4.3.2 Run-And-Tumble

An experiment, analogous to the one carried out in the case of diffusion, can be done for the RTP case. We use the same set-up for the initial conditions and time interval but now the particles obey the run-and-tumble dynamics as explained in section 4.1. The characteristics of the dynamics here are an average rate of switching $\alpha = 0.5$ and a velocity $v_0 = 1$, so an effective diffusion coefficient $D_{\text{eff}} = v_0^2/2\alpha = 1$. This results in a distribution plotted in figure 11. We can again fit the relative amounts of all the different flux values to compare with the analytical results given by combining (3.34) and (3.16), as done for diffusion in the previous section.

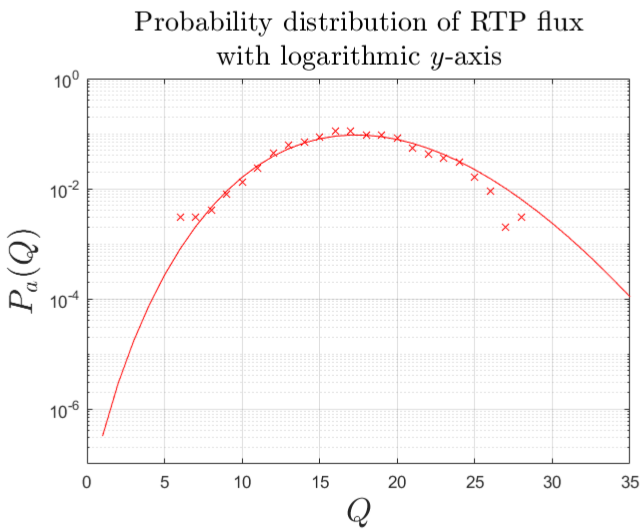
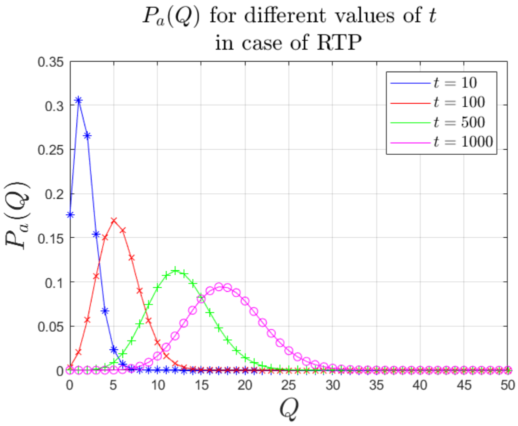


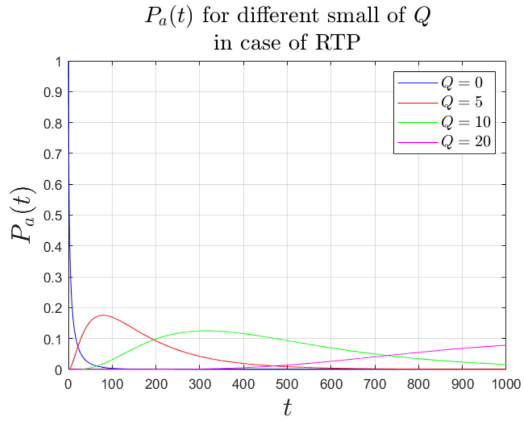
Figure 11: A semi-log plot of the probability distribution $P_a(Q,t)$ vs. the flux Q up to a time $t = 1000$ for RTP. The average rate of change used is $\alpha = 0.5$, the velocity $v_0 = 1$ ($D_{\text{eff}} = 1$). The red crosses indicate the different flux values and their corresponding numerical probabilities as obtained by the Monte Carlo simulations. The solid red line is the analytical predicted distribution.

To visualize the probability of the flux at a certain time we plot $P_a(Q,t)$ vs. Q at different values for t. This is done in figure 12a. These distributions are very similar to the ones in figure 10a. The peak of the curve broadens and curve itself flattens as time increases.

On the other hand, we can examine the probability distribution for different flux values in time. These are plotted in figure 12b and again look very similar to the diffusion case. The peak also shifts to the right and flattens as the flux increases. The probability of having a zero flux at times $t > 0$ nearly vanishes.



(a) Caption



(b)

Figure 12: In both pictures we consider the RTP case with an effective diffusion coefficient $D_{\text{eff}} = 1$. **Left:** Plots of the probability distribution of the flux at different times. The different possible flux values are marked and their corresponding probability is read from the vertical axis. **Right:** Probability distribution of different small flux values in time.

4.3.3 Comparison

Finally we can compare the distribution for the flux of both cases on one single plot (figure 13). We do this by taking data from the Monte Carlo simulations we explained earlier. These simulations are again done with 100 particles uniformly distributed across the interval $[-100, 0]$, such that the particle density is $\rho = 1$. These particles move according to the discussed dynamics. After a time $t = 1000$, the flux given by both of these dynamics is noted and the same simulation is repeated. This is done 1000 times. Once again, the relative amounts of each flux value are fitted. When inspecting figure 13, both analytical predicted distributions seem to coincide, although the numerical probabilities in the RTP case are sometimes slightly higher than the ones in the diffusion case for the same flux value.

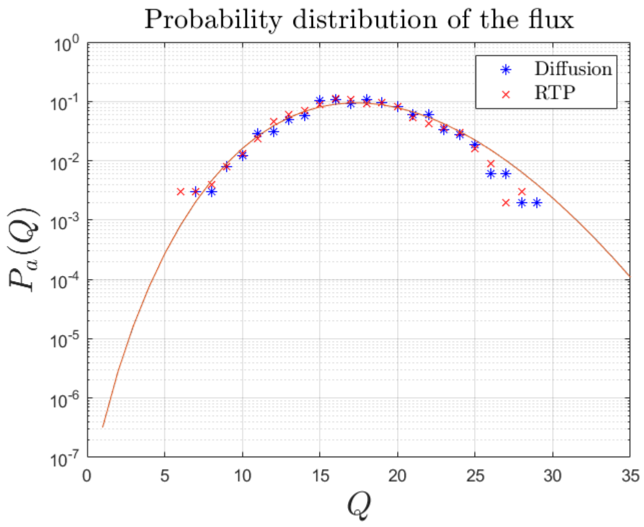


Figure 13: A comparison of the probabilities of the different flux values for diffusive particles and RTP up to a time $t = 1000$ with $D = D_{\text{eff}} = 1$. The blue asterisks and the red crosses indicate the different flux values and their corresponding numerical probabilities for diffusion and RTP respectively. The solid lines represent the analytical predicted distributions.

5 Conclusion

We have proposed a general way of calculating the probability distribution of the flux of non-interacting particles in one dimension for any dynamics, starting from step-initial conditions. At time $t = 0$, all the particles are on the left of the origin and uniformly distributed. We consider the probability distribution of the flux up to time t. This probability distribution is Poisson distributed with a mean and variance $\mu(t)$. The function $\mu(t)$ depends solely on the dynamics of the particle. For different dynamics, the stochastic equation of motion, the Langevin equation needs to be obtained in order to get the probability of the position of the particle. A double integral of this probability then gives the function $\mu(t)$.

In this paper, diffusion and run-and-tumble dynamics are both discussed and compared to get a better understanding on how a RTP behaves. Both for diffusion and RTP, $\mu(t)$ is calculated (see Eq.(3.26) and Eq. (3.34) respectively). These function are plotted and they occur to be very similar, therefore we could make an educated guess that for the large time limit, $\mu(t)_{\text{RTP}}$ is equal to $\mu(t)_{\text{diff}}$. For the small time limit, we know that $\mu(t)_{\text{RTP}}$ behaves linearly.

We have verified our analytical predictions by using numerical simulations. The numerical data of the probability distribution of the flux, obtained via the Monte-Carlo method, matches very well with the analytical results, both for diffusion and RTP-dynamics. The probability distribution for different times will always have the form of a Poisson distribution, as expected. As time increases, the peak of the probability in function of the flux broadens and the curve flattens. When visualizing the probability in function of the time for different fluxes, this peak also shifts to the right and flattens as the flux is increased. The probability of having a zero flux at time $t > 0$ drops drastically to a near zero probability.

From the numerical comparison between the RTP and the diffusion, we can conclude that in the small time limit, RTP and diffusive particles behave differently. Comparing $\mu(t)_{\text{diff}}$ with $\mu(t)_{\text{RTP}}$ in the small time limit we can clearly see that $\mu(t)_{\text{diff}}$ increases more rapidly and $\mu(t)_{\text{RTP}}$ behaves more linearly. In the large time limit, an RTP behaves like a diffusion particle, with an effective diffusion coefficient $D_{\text{eff}} = v_0/2\alpha$. When comparing the numerical results of the diffusive particle and RTP graphically, the probability distribution of the two different fluxes seem to coincide. However, if we look more into detail, we can see that the probability of finding a certain flux value at a given moment in time for the RTP is slightly higher than that of the diffusive case.

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