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Path integrals for boundaries in diffusion and quantum mechanics

by

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Abstract

Diffusion and quantum mechanics with boundary conditions arise naturally in various situations in physics. While reflecting and absorbing boundaries are well mathematically described, intermediate scenarios are not that clear. Consider a reflective boundary which is removed for a time δ and subsequently reinstated. First, we place a Brownian particle at one side of this barrier and study its path-integral propagator. We obtained a closed expression for the particle's probability of being before or after the barrier at a certain time. We then consider the same barrier, but when the removing time is unforeseen, so the particle could cross to the other side at some time within a known interval $[0, T]$. A path-integral propagator is computed, and it is shown numerically that the limit to the exact path integral is convergent. Finally, we consider a quantum particle in the presence of a reflective barrier removed at $t = \Delta t_1$ for a time δ and then reinstated. We propose a path-integral propagator for this process and show that the corresponding wave function satisfies the Schrödinger equation.

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Contents

Chapter 1

Introduction

The purpose of this work is to study the propagation of Brownian and quantum particles in the presence of certain time-dependent barriers. Since both quantum mechanics and diffusion share similar mathematical descriptions, and accept a path integral formulation, we aim to describe a physical scenario that works for the two cases.

We begin discussing the Brownian particle which is a well-known stochastic process. A system is considered stochastic if its time evolution is subject to random forces, leading to the study of probabilities instead of deterministic predictions. In 1827, while studying pollen grains suspended in water under a microscope, the botanist Robert Brown observed tiny particles, ejected by the pollen grains, doing a jittery motion [1]. He was able to rule out that the motion was life-related by repeating the experiment with particles of inorganic matter, although its origin was yet to be explained. At the time, the theory of atoms and molecules was controversial to physicists, so when Albert Einstein in one of his 1905 papers [2] brought the solution of the problem to their attention, the idea of microscopic structures causing effects on the movement of macroscopic particles became more plausible, giving rise to a more formal and mathematical study of diffusion.

There are many diffusion processes in nature that are studied in terms of Brownian motion. A few examples are the diffusion of pollutants through the atmosphere [3, 4], the motion of a massive body (such as a star or a black hole) as it responds to gravitational forces from surrounding stars [5, 6], the diffusion of calcium through bone tissue in living organisms

[7, 8], among others. In particular, diffusion with boundary conditions is widely studied in the literature [9, 10, 11].

Diffusion with absorbing boundary conditions

In this processes, particles are removed or "killed" from the system when they reach the boundary. These boundaries do not conserve the system's particle number, allowing to define the survival and first-hitting-time probabilities [12, 13]. The calculation of these quantities is relevant in probability theory and has had immediate applicability in a myriad of problems: spreading of diseases [14], animal or human movement [15], neuron firing dynamics [16] or diffusion in bounded domains [17]. This type of system is readily modeled by a diffusion equation with Dirichlet boundary conditions.

Diffusion with reflecting boundary conditions

Reflecting boundaries arise when no-flux is assumed to pass through the boundary, so the particles bounce off upon arrival. This applies to most diffusion processes in finite volumes, where unlike the previous case, the number of particles in conserved in time so no survival probability is defined. Further applications are queuing models experiencing heavy traffic [18] as proposed by Kingman [19] and proven by Iglehart and Whitt [20].

These systems are typically modeled by a diffusion equation with Neumann boundary conditions [9].

Neither reflecting nor absorbing

However, not all processes fall into one of the previous categories. We can think of a time-dependent boundary, which is reflecting for a certain time until suddenly, allows particle passage to then become reflecting again. This allows us to define a survival probability, which is slightly different from the usual definition since this boundary accretes particles for a finite amount of time. In order to solve the problem, it is useful to introduce a wall-operator, which is in charge of removing and reinstate the boundary. Making reference to Maxwells' famous thought experiment [21], this operator will be referred to the "demon".

We first examine the case of a reflective wall at $x = 0$ that is removed at $t = \Delta t_1$ for a time δ and then is restored. The relevant question is: What is the probability of finding the particle before (or after) the barrier at a time T?. We obtain the path integral propagator for this process and find a closed expression for the probability in the entire domain before and after the wall. Further, we show that for short opening time δ, the probability of the particle to be after the barrier is $O(\delta^{1/2})$.

We then study a reflective wall at $x = 0$ removed at an **unknown** time during an interval δ and subsequently reinstated; the uncertain time of removal is interpreted as the demon's action on the wall. The removal of the wall is achieved by replacing one microscopic reflecting-wall propagator for a free particle propagator in the discrete path integral, and the demon is introduced by summing over the possible removal times. The probability density is computed along with the Shannon entropy of the system.

In section 3.2 we consider a quantum particle in the presence of a reflective wall at $x = 0$, removed at $t = \Delta t_1$ for a time δ and then restored. Marchewka and Schuss [22] already studied the propagation of quantum particles when a wall is removed and reinstated using path integrals. They found that the probability propagated across the boundary in time Δt is $O(\Delta t^{3/2})$, which is a Zeno Effect [23]. Our scenario is slightly different because the boundary is not removed instantaneously but after a time Δt_1. In this context, it is shown that the probability propagated across the boundary is $O(\Delta t_1^{-3})$ for $\Delta t_1 \gg \frac{m x_0^2}{2\hbar}$.

The structure of this work is the following: the first chapter is devoted to theoretical framework, where diffusion is first presented as a result of a random walk and is then re-discovered in the context of differential equations. Further, we obtain the diffusion and Schrödinger propagators for the free particle and the reflective wall. Section 3.1 contains the main calculations and results obtained for the Brownian particle, and Section 3.2 addresses the quantum particle in the same scenario of Sec. 3.1.1.

Chapter 2

Theory

2.1 Random walk, diffusion and Brownian motion

A random walk is a stochastic process consisting of an idealized path performed by a succession of random steps [24]. It is relevant in mathematics, physics, biology, and finance [25, 26, 27]. In particular, it can denote the path traced by a Brownian particle as it travels in a liquid [28]. By having the probability of each result in each step (for example, right / left, up / down), we can obtain the probability of finding the particle in a given position after N steps.

Since real-life particles do not travel by jumping in steps, we would like to have a continuous model, that is, a model where the steps are so small that the particle can be anywhere in space and time. In this section, we will show that the probability density of a continuous random walk satisfies a differential equation called diffusion equation [29].

Consider a walker which moves along the x-axis by steps. Each step has the length h and time duration τ. The walker in each step can move either h to the right (event R) or h to the left (event L).

The probability distribution of the number of successes in a sequence of N independent experiments, each with its own boolean-valued outcome: left (with probability p) or right (with probability $q = 1 - p$), is given by the binomial distribution

$$P_N(k) = \binom{N}{k} p^k q^{N-k} \tag{2.1}$$

where k are the steps to the right and $N - k$ to the left. The binomial theorem states

$$(pu + q)^N = \sum_{k=0}^{N} \binom{N}{k} u^k p^k q^{N-k} \tag{2.2}$$

which leads to

$$\sum_{k=0}^{N} P_N(k) = (p + q)^N = 1. \tag{2.3}$$

where we verify that $P_N(k)$ is normalized to one.The expectation value or first moment of k is

$$\begin{aligned}
\langle k \rangle = \sum_{k=0}^{N} k P_N(k) &= \sum_{k=0}^{N} k \left[\binom{N}{k} u^k p^k q^{N-k} \right]_{u=1} \\
&= \sum_{k=0}^{N} \left[u \frac{\mathrm{d}}{\mathrm{d}u} \binom{N}{k} u^k p^k q^{N-k} \right]_{u=1} \qquad (2.4) \\
&= \left[u \frac{\mathrm{d}}{\mathrm{d}u} \sum_{k=0}^{N} \binom{N}{k} u^k p^k q^{N-k} \right]_{u=1} \qquad (2.5) \\
&= \left[u \frac{\mathrm{d}}{\mathrm{d}u} (pu + q)^N \right]_{u=1} = Np, \qquad (2.6)
\end{aligned}$$

similarly for the second moment

$$\begin{aligned}\left\langle k^2\right\rangle = \sum_{k=0}^{N} k^2 P_N(k) &= \sum_{k=0}^{N} k^2 \left[\binom{N}{k} u^k p^k q^{N-k}\right]_{u=1} \\ &= \sum_{k=0}^{N} \left[\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^2 \binom{N}{k} u^k p^k q^{N-k}\right]_{u=1} && (2.7) \\ &= \left[\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^2 \sum_{k=0}^{N} \binom{N}{k} u^k p^k q^{N-k}\right]_{u=1} && (2.8) \\ &= \left[\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^2 (pu+q)^N\right]_{u=1} = Np + Np^2(N-1). && (2.9)\end{aligned}$$

Now we compute the variance as follows

$$\sigma^2 = \left\langle k^2\right\rangle - \left\langle k\right\rangle^2 = Np(1-p) = Npq \tag{2.10}$$

which is a measure of the width of the distribution. Let $m = 2k - N$ be the walker's position after N steps, its expectation value is

$$\left\langle m\right\rangle = 2\left\langle k\right\rangle - N = N(2p-1) = N(p-q) \tag{2.11}$$

and the second moment

$$\left\langle m^2\right\rangle = 4\left\langle k^2\right\rangle - 4N\left\langle k\right\rangle + N^2 = 4\sigma^2 + \left\langle m\right\rangle^2 \tag{2.12}$$

which leads to a variance

$$\sigma_m^2 = \left\langle m^2\right\rangle - \left\langle m\right\rangle^2 = 4\sigma^2 = 4Npq. \tag{2.13}$$

When the squared displacement is proportional to time (or the number of steps N), we call this a **free diffusion** process.

Introducing the real displacement $x = mh$ and the time $t = N\tau$ we have

$$\sigma_x^2 = \left\langle x^2\right\rangle - \left\langle x\right\rangle^2 = h^2\left(\left\langle m^2\right\rangle - \left\langle m\right\rangle^2\right) = 4pqNh^2 = 4pqt\frac{h^2}{\tau} = 2Dt \tag{2.14}$$

where $D \equiv \frac{2h^2pq}{\tau}$. Equation (2.14) is the well-known expression derived by Einstein for the mean squared displacement of a Brownian particle [2]. The average position of the walker is

$$\langle x \rangle = h \langle m \rangle = N(p-q)h = vt \tag{2.15}$$

which defines the drift velocity $v = (p-q)\frac{h}{\tau}$. For a symmetric walk where $p = q = \frac{1}{2}$, the drift velocity and the average position are zero. In such case the probability (2.1) becomes

$$P(m,N) = \frac{2^{-N}N!}{\frac{(m+N)!}{2!}\frac{(N-m)!}{2!}}. \tag{2.16}$$

which satisfies

$$P(m,N+1) = \frac{1}{2}P(m+1,N) + \frac{1}{2}P(m-1,N). \tag{2.17}$$

We re-write (2.17) as

$$\frac{P(m,N+1)-P(m,N)}{\tau} = \frac{h^2}{2\tau}\frac{P(m+1,N)-2P(m,N)+P(m-1,N)}{h^2} \tag{2.18}$$

and after the substitution

$$D = \frac{h^2}{2\tau}, \tag{2.19}$$

we find

$$\frac{P(m,N+1)-P(m,N)}{\tau} = D\frac{P(m+1,N)-2P(m,N)+P(m-1,N)}{h^2}, \tag{2.20}$$

taking the limit $\tau \to 0$, $h \to 0$ we get to the form of the diffusion (heat) equation

$$\frac{\partial P}{\partial \tau} = D\frac{\partial^2 P}{\partial x^2}. \tag{2.21}$$

On the other hand, when N is large we can use Stirling's formula

$$\log(n!) = \left(n + \frac{1}{2}\right)\log(n) - n + \frac{1}{2}\log(2\pi) \tag{2.22}$$

to simplify equation (2.16). We obtain

$$\begin{aligned}\log P \approx{}& \left(N + \frac{1}{2}\right)\log N - \frac{1}{2}(N+m+1)\log\left[\frac{N+m}{2}\right] - \frac{1}{2}(N-m+1)\log\left[\frac{N-m}{2}\right] \\ &- \frac{1}{2}\log 2\pi - N\log 2,\end{aligned} \tag{2.23}$$

now write

$$\frac{N \pm m}{2} = \frac{N}{2}\left(1 \pm \frac{m}{N}\right) \tag{2.24}$$

and expand for $m \ll N$ as follows

$$\log\left(1 \pm \frac{m}{N}\right) \approx \pm\frac{m}{N} - \frac{m^2}{2N^2}. \tag{2.25}$$

Equation (2.23) now becomes

$$\begin{aligned}\log P \approx{}& \left(N + \frac{1}{2}\right)\log N - \frac{1}{2}(N+m+1)\left[\log\frac{N}{2} + \frac{m}{N} - \frac{m^2}{2N^2}\right] - \\ &\frac{1}{2}(N-m+1)\left[\log\frac{N}{2} - \frac{m}{N} - \frac{m^2}{2N^2}\right] - \frac{1}{2}\log 2\pi - N\log 2\end{aligned} \tag{2.26}$$

Simplifying we obtain

$$\log P \approx -\frac{1}{2}\log N + \log 2 - \frac{1}{2}\log 2\pi - \frac{m^2}{2N} \tag{2.27}$$

which leads to

$$P(m,N) \approx \sqrt{\frac{2}{\pi N}}\, e^{-\frac{m^2}{2N}}. \tag{2.28}$$

Since the problem is translational invariant, if the walker starts at a point different from zero, say, $m = m_0$, the solution changes only by a shift

$$P(m, m_0, N) \approx \sqrt{\frac{2}{\pi N}} e^{-\frac{(m-m_0)^2}{2N}}. \tag{2.29}$$

If every step has length l and each step take a time τ then the initial position of the particle will be $x_0 = m_0 l$, the final position $x = ml$ and the time of the Nth step $t = N\tau$. Re-writting $P(m, m_0, N)$ we have

$$P(x, x_0, t) = \sqrt{\frac{1}{4\pi Dt}} \left(e^{-\frac{(x-x_0)^2}{4Dt}} \right) \tag{2.30}$$

2.2 Random walk with reflecting barrier

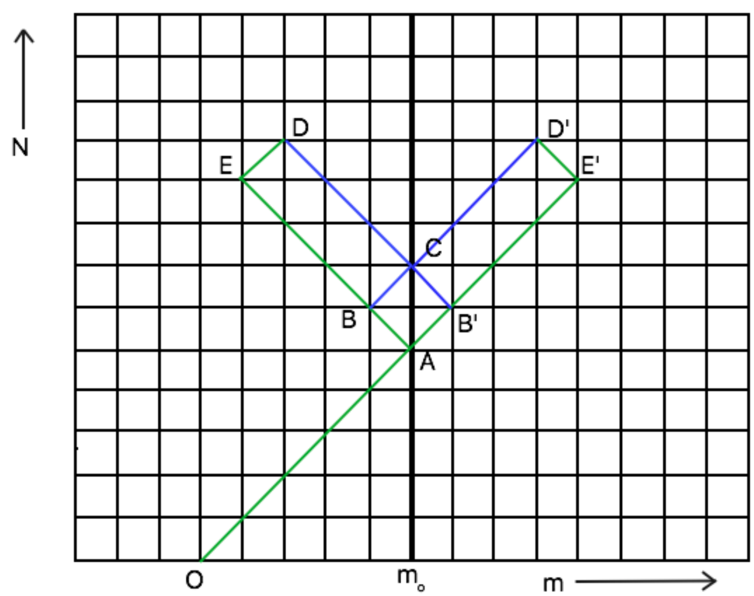


Figure 2.1

Consider a barrier at $m = m_0$ such that the particle has probability 1 to turn left when reaching it. Naturally, trajectories that otherwise would not get to a certain point now will because of the reflection, causing the probability to increase. Consider the $N - m$ plane of Figure 2.1, where N are the steps, and m is the position of the particle. In the absence of a barrier, the probability that a particle arrives at m after N steps is given by (2.16). Take, for example, the green path; without barrier, it would count once, but now, with a barrier, the step AB is rather obligated, so, a trajectory that would otherwise prefer B' (without barrier) has now to be added to the probability. Note that for every trajectory leading to the point m after hitting the barrier once, there is exactly one trajectory leading to the image point after a single reflection. Conversely, for every trajectory leading to the image point that cross the barrier once, only one trajectory leads to m after a single reflection. Thus, there is a one-to-one correspondence between a trajectory and its reflected companion. The probability will contain the trajectories without barrier plus the trajectories leading to the image point

$$P_W(m,N) = P(m,N) + P(2m_0 - m, N) \tag{2.31}$$

where $P(m,N)$ is given by (2.16). If we shift the problem such as the barrier is at $m = 0$ we have, for $N \gg m$

$$P_W(m,N) = \sqrt{\frac{2}{\pi N}} \left(e^{-\frac{(m-m_0)^2}{2N}} + e^{\frac{(m+m_0)^2}{2N}} \right) \tag{2.32}$$

which in the continuous limit $x = mh$, $t = N\tau$ $h, \tau \to 0$ becomes

$$P_W(x,t) = \sqrt{\frac{1}{4\pi Dt}} \left(e^{-\frac{(x-x_0)^2}{4Dt}} + e^{-\frac{(x+x_0)^2}{4Dt}} \right) \tag{2.33}$$

with D the diffusion coefficient defined in (2.19). Just as (2.30) is a solution to the the diffusion equation (2.21), $P_W(x,t)$ is too with boundary conditions

$$J(x=0,t) = \left[\frac{\partial P_W(x,t)}{\partial x} \right]_{x=0} = 0 \tag{2.34}$$

where $J(x,t)$ is the current at position x at time t. This is a reflecting boundary condition, and states that there is no particle flux through the wall.

2.3 Computing propagators

Many natural phenomena are described by differential equations, from quantum to classical physics. In particular, two well-known differential equations are the diffusion and Schrödinger equations; both describe the time evolution of probability density. One can obtain the probability density at any time by knowing a quantity called Green's function, which is related to the differential operator of the equation and propagates the probability function in time. In this section, we will calculate the Green's function of the diffusion and Schrödinger equations. In diffusion, we shall find the same results as in our discussion on random walks, but as R. Feynman said: "there is a pleasure in recognizing old things from a new point of view."

2.3.1 Green's Function

In particular, if L is a linear differential operator, acting at a point (x_0, t_0), we define the Green's function $G(x, x_0; t, t_0)$ of the operator L as:

$$L(x,t)G(x,x_0;t,t_0) = \delta(x - x_0)\delta(t - t_0). \tag{2.35}$$

If we multiply (2.35) by some function $u(x_0, t_0)$ and integrate in x_0

$$\begin{aligned} L(x,t)\int dx_0\ G(x,x_0;t,t_0)u(x_0,t_0) &= \delta(t-t_0)\int dx_0\ \delta(x-x_0)u(x_0,t_0) \\ &= \delta(t-t_0)u(x,t_0), \end{aligned} \tag{2.36}$$

and define

$$u(x,t) = \int dx_0\ G(x,x_0;t,t_0)u(x_0,t_0), \tag{2.37}$$

we are left with

$$L(x,t)u(x,t) = \delta(t-t_0)u(x,t_0). \tag{2.38}$$

For $t \neq t_0$, (2.38) is

$$L(x,t)u(x,t,t_0) = 0, \tag{2.39}$$

which is a linear homogeneous differential equation. If we know the Green's function $G(x, x_0; t, t_0)$ and the initial condition $u(x_0, t_0)$, the solution is given by (2.37).
For $t = t_0$ we require that

$$\lim_{t \to t_0} G(x, x_0; t, t_0) = \delta(x - x_0). \tag{2.40}$$

Conversely, if we consider an initial impulse $u(x_0, t_0) = \delta(x' - x_0)$ in equation (2.37), then $u(x,t) = G(x, x'; t, t_0)$, which allows us to interpret the Green's function as the system's response to an impulse. On the other hand, equation (2.37) shows that the Green's function plays the role of propagation between the function u at some time, to another. That is why in some contexts, Green's functions are called **propagators**.

2.3.2 The diffusion propagator

Now we compute the propagator for a diffusion process. The result is obtained from the Green's function defining differential equation. A fluid of density $\rho(x,t)$ tends to flow from a point where the density is high, towards a region of low density. The current J is therefore assumed to be proportional to the gradient of the density:

$$\mathbf{J} = -D\frac{\partial \rho}{\partial x}, \tag{2.41}$$

where D is the so-called diffusion constant. If we combine (2.41) with the continuity equation, we obtain the diffusion equation

$$\left(\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right)\rho(x,t) = 0. \tag{2.42}$$

Now we want to compute the Green's function $G(x, x_0; t, t_0)$ of (2.64) in an infinite one-dimensional region. The defining differential equation for G is

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} - D\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) G(x, x_0; t, t_0) = 4\pi\delta(x - x_0)\delta(t - t_0) \tag{2.43}$$

Since the Green's function depends only on the differences, we define $r = x - x_0$, $\tau = t - t_0$. We write down the Fourier transform of the Green's function

$$G(r, \tau) = \frac{1}{2\pi}\int \mathrm{d}k\ e^{ikr} g(k, \tau) \tag{2.44}$$

We insert (2.44) into the defining equation (2.43) and use the Fourier representation of the δ function to obtain

$$\frac{\mathrm{d}g}{\mathrm{d}\tau} + Dk^2 g = 4\pi\delta(\tau). \tag{2.45}$$

This differential equation has the following causal solution

$$g(k, \tau) = 4\pi D e^{-k^2\tau D}\Theta(\tau) \tag{2.46}$$

if we insert (2.46) in (2.44), we obtain a Gaussian integral (Appendix A)

$$G(r, \tau) = \frac{1}{2\pi}\int \mathrm{d}k\ e^{ikr} 4\pi D e^{-k^2\tau D}\Theta(\tau) \tag{2.47}$$

leading to the Green's function

$$G(r, \tau) = \frac{1}{\sqrt{4\pi D\tau}} e^{-\frac{r^2}{4D\tau}}\Theta(\tau). \tag{2.48}$$

which is the same function we obtained for the probability distribution in a continuous random walk (2.30).

2.3.3 The Schrödinger propagator

The Schrödinger equation is

$$-\hbar^2 \frac{\partial^2 \Psi(x,t)}{\partial x^2} = i\hbar \frac{\partial \Psi(x,t)}{\partial t}, \tag{2.49}$$

if U_E is an eigenstate of the Hamiltonian

$$-\hbar^2 \frac{\mathrm{d}^2 \Psi(x,t)}{\mathrm{d}x^2} = E U_E, \tag{2.50}$$

then we can write down

$$\Psi(x,t) = \sum_E A_E(t) U_E(x) \tag{2.51}$$

$$A_E(t) = \int U_E^*(x) \Psi(x,t) \mathrm{d}x. \tag{2.52}$$

Now we insert (2.51) in (2.49) obtaining

$$-\hbar^2 \sum_E A_E(t) \left(\frac{\mathrm{d}^2 U_E(x)}{\mathrm{d}x^2} \right) = i\hbar \sum_E U_E(x) \left(\frac{\mathrm{d}A_E(t)}{\mathrm{d}t} \right), \tag{2.53}$$

which, using equation (2.50) and the ortonormality of U_E, gives a differential equation for $A_E(t)$

$$E A_E(t) = i\hbar \frac{\mathrm{d}A_E(t)}{\mathrm{d}t} \tag{2.54}$$

with solution

$$A_E(t) = A_E(t') e^{i\frac{E(t'-t)}{\hbar}}. \tag{2.55}$$

Inserting (2.55) in (2.51) and using (2.52) we have

$$\begin{aligned}\Psi(x,t) &= \sum_E A_E(t')e^{i\frac{E(t'-t)}{\hbar}}U_E(x)\\ &= \sum_E \left(\int U_E^*(x')\Psi(x',t')\mathrm{d}x'\right)e^{i\frac{E(t'-t)}{\hbar}}U_E(x)\\ &= \int\left(\sum_E U_E^*(x')U_E(x)e^{i\frac{E(t'-t)}{\hbar}}\right)\Psi(x',t')\mathrm{d}x',\end{aligned} \tag{2.56}$$

where, by comparing with the convolution property (2.37), we have found the eigenmode expansion for the Green's function

$$G(x,t;x',t') = \sum_E U_E^*(x')U_E(x)e^{i\frac{E(t'-t)}{\hbar}}. \tag{2.57}$$

Using plane waves for the eigenfunctions

$$U_E(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{px}{\hbar}}, \tag{2.58}$$

we have

$$G(x,t;x',t') = \frac{1}{2\pi\hbar}\int e^{i\frac{p(x-x')}{\hbar}}e^{-i\frac{p^2(t-t')}{2m\hbar}}\mathrm{d}p, \tag{2.59}$$

working on the argument of the exponential, we finally get to

$$G(x,t;x',t') = \sqrt{\frac{m}{2\pi\hbar iT}}e^{\frac{im}{2\hbar T}(x-x')^2} \tag{2.60}$$

with $T = t - t'$. This is the unrestricted, free Green's function that describes the propagation into the future as well as back into the past. The retarded and advanced Greens functions are

$$G^+(x,t;x',t') = \Theta(t-t')G(x,t;x',t') \tag{2.61}$$

$$G^-(x,t;x',t') = -\Theta(t'-t)G(x,t;x',t') \tag{2.62}$$

Note that the transformation $T \to -i\tau$ changes the Green's function (2.60) into the Green's function for the diffusion equation.

2.3.4 The reflective wall

Diffusion equation

We aim to describe diffusion in half space with reflecting boundary conditions. The latter means that there is no particle flux across the boundary. If the current J is proportional to the gradient of particle density as stated in (2.41), then the boundary condition will be

$$\lim_{x\to 0} J(x,t) = \frac{\mathrm{d}\rho(x,t)}{\mathrm{d}x} = 0 \tag{2.63}$$

with the boundary located in $x = 0$. In particular, we want to obtain the Green's function $K_W(x, x_0; t, t_0)$ for the diffusion equation with such a boundary condition, i.e, a solution for

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} - D\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) K_W(x, x_0; t, t_0) = 0. \tag{2.64}$$

with initial condition

$$\lim_{t\to t_0} K_W(x, x_0; t, t_0) = \delta(x - x_0) \tag{2.65}$$

and boundary condition

$$\lim_{x\to 0} \frac{\mathrm{d}K_W(x, x_0; t, t_0)}{\mathrm{d}x} = 0. \tag{2.66}$$

The propagator that fulfills all those requirements is

$$K_W(x, x_0, \tau) = \left(\frac{1}{4\pi\tau D}\right)^{\frac{1}{2}} \left(e^{-\frac{(x-x_0)^2}{4D\tau}} + e^{-\frac{(x+x_0)^2}{4D\tau}}\right), \tag{2.67}$$

where $\tau = t - t_0$. This propagator represents the probability density of a Brownian particle to propagate from (x_0, t_0) to (x, t) in the presence of a reflective barrier at $x = 0$, and is the same function we encounter in a continuous random walk with a reflective barrier (2.33).

Quantum mechanics

In this section we will compute the quantum mechanical propagator of a particle confined to the half plane. The completeness relation reads

$$1 = \int_0^\infty |r\rangle \langle r| \, \mathrm{d}r \tag{2.68}$$

we want to compute

$$\langle r_b, t_b | r_a, t_a \rangle = \langle r_b | \, e^{-i\frac{\hat{H}(t_b - t_a)}{\hbar}} \, |r_a\rangle \tag{2.69}$$

$$= \langle r_b | \prod_{n=1}^{N-1} e^{-i\frac{\hat{H}\epsilon}{\hbar}} \, |r_a\rangle \, . \tag{2.70}$$

We factorize into many time slices

$$\langle r_b, t_b | r_a, t_a \rangle = \prod_{n=1}^{N} \left[\int_0^\infty \mathrm{d}r_n \right] \prod_{j=1}^{N+1} \langle r_j | \, e^{-i\frac{\hat{H}\epsilon}{\hbar}} \, |r_{j-1}\rangle \, , \tag{2.71}$$

and as $H(\hat{p_j}) = H(-i\hbar\partial_{r_j})$, we have

$$\langle r_b, t_b | r_a, t_a \rangle = \prod_{n=1}^{N} \left[\int_0^\infty \mathrm{d}r_n \right] \prod_{j=1}^{N+1} e^{-\frac{i\epsilon}{\hbar} H(-i\hbar\partial_{r_j})} \, \langle r_j | r_{j-1} \rangle \tag{2.72}$$

The spectral representation of the transition element $\langle r | r' \rangle$ is

$$\langle r | r' \rangle = \int_{-\infty}^{\infty} \mathrm{d}k \, \langle r | k \rangle \, \langle k | r' \rangle \, , \tag{2.73}$$

we insert the $\langle r|k\rangle$ corresponding to a solution whose boundary condition is to vanish at $r = 0$

$$\langle r | k \rangle = \frac{1}{\sqrt{4\pi}} \left(e^{ikr} - e^{-ikr} \right) . \tag{2.74}$$

Replacing in Equation (2.73) we have

$$\begin{aligned}\langle r | r' \rangle &= \frac{1}{4\pi}\int_{-\infty}^{\infty} \mathrm{d}k \left(e^{ikr} - e^{-ikr}\right)\left(e^{-ikr'} - e^{ikr'}\right) \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \left(e^{ik(r-r')} - e^{ik(r+r')}\right) \\ &= \delta(r-r') - \delta(r+r'), \end{aligned} \tag{2.75}$$

then, replacing $p = \hbar k$

$$\begin{aligned} e^{-\frac{i\epsilon}{\hbar}H(-i\hbar\partial_{r_j})}\langle r_j | r_{j-1}\rangle &= e^{-\frac{i\epsilon}{\hbar}H(-i\hbar\partial_{r_j})}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi\hbar}\left(e^{i\frac{p}{\hbar}(r_j-r_{j-1})} - e^{i\frac{p}{\hbar}(r_j+r_{j-1})}\right) \\ &= \int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi\hbar}e^{-\frac{i\epsilon}{\hbar}H(p)}\left(e^{i\frac{p}{\hbar}(r_j-r_{j-1})} - e^{i\frac{p}{\hbar}(r_j+r_{j-1})}\right). \end{aligned} \tag{2.76}$$

It can be seen that, for simplicity, we can work on the amplitude $\langle r_b, t_b | r_a, t_a\rangle$ with zero Hamiltonian and at the end add $-\frac{i\epsilon}{\hbar}H(p)$ to the exponent inside the momentum integral. Equation (2.75) can be re-written as follows

$$\langle r | r' \rangle = \sum_{x=\pm r}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi\hbar}\exp\left(\frac{i}{\hbar}p(x-x') + i\pi(\sigma(x) - \sigma(x'))\right)\Bigg|_{x'=r'} \tag{2.77}$$

where

$$\sigma(x) := \Theta(-x). \tag{2.78}$$

The amplitude with zero Hamiltonian is

$$\langle r_b, t_b | r_a, t_a\rangle_0 = \langle r_a | r_b\rangle \tag{2.79}$$

we factorize into many time slices

$$\langle r_b, t_b | r_a, t_a\rangle_0 = \prod_{n=1}^{N}\left[\int_0^{\infty} dr_n\right]\prod_{i=1}^{N+1}\langle r_i | r_{i-1}\rangle, \tag{2.80}$$

by inserting equation (2.77) we obtain

$$\langle r_b, t_b | r_a, t_a \rangle_0 = \prod_{n=1}^{N} \left[\int_0^\infty dr_n \right] \prod_{j=1}^{N+1} \left[\sum_{x_j = \pm r_j} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_j}{2\pi\hbar} \right] \exp\left(\frac{i}{\hbar} p(x_j - x_{j-1}) + i\pi(\sigma(j_j) - \sigma(x_{j-1})) \right), \tag{2.81}$$

for every "n" we will basically have an integral of the type

$$\int_0^\infty \mathrm{d}r \, (f(r) + f(-r)) = \int_{-\infty}^{\infty} \mathrm{d}x f(x) \tag{2.82}$$

only the last sum cannot be accommodated in this way because there is no integral over r_{N+1}. We get to

$$\langle r_b, t_b | r_a, t_a \rangle_0 = \sum_{x_b = \pm r_b} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} dx_n \right] \prod_{j=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_j}{2\pi\hbar} \right] \exp\left(\sum_{k=1}^{N+1} \frac{i}{\hbar} p(x_k - x_{k-1}) + i\pi(\sigma(x_k) - \sigma(x_{k-1})) \right), \tag{2.83}$$

where we have set $x_{N+1} = x_b$, $r_{N+1} = r_b$. Now the integration measure is the usual for the path integral without constraints. In the continuum limit, the exponent corresponds to an action

$$A_0^\sigma[p, x] = \int_{t_a}^{t_b} \mathrm{d}t \, (p\dot{x} + \hbar\pi\partial_t \sigma(x)) = A_0(p, x) + A_{topol}^\sigma. \tag{2.84}$$

Consider now a free particle in the right half space with the Hamiltonian

$$H = \frac{p^2}{2m} \tag{2.85}$$

as we stated before, the Hamiltonian can be added to the action without a problem, so we have

$$A[p, x] = \int_{t_a}^{t_b} \mathrm{d}t \left(p\dot{x} - \frac{p^2}{2m} + \hbar\pi\partial_t \sigma(x) \right), \tag{2.86}$$

and the topological term is

$$A^{\sigma}_{topol} = \hbar\pi \left(\sigma(x_b) - \sigma(x_a)\right). \tag{2.87}$$

The propagator will be

$$\langle r_b, t_b | r_a, t_a \rangle = \sum_{x_b = \pm r_b} \int Dx \int \frac{Dp}{2\pi\hbar} \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t \ \left[p\dot{x} - \frac{p^2}{2m} + \hbar\pi\left(\sigma(x_b) - \sigma(x_a)\right)\right]\right), \tag{2.88}$$

the integrals are carried out in the same way as for a free particle since the last is a pure boundary term. The result is

$$\begin{aligned}\langle r_b, t_b | r_a, t_a \rangle &= \sum_{x_b = \pm r_b} \sqrt{\frac{m}{2\pi i (t_b - t_a)}} \exp\left[\frac{im}{2\hbar}\frac{(x_b - x_a)^2}{t_b - t_a} + i\pi\left[\sigma(x_b) - \sigma(x_a)\right]\right] \\ &= \sqrt{\frac{m}{2\pi i (t_b - t_a)}} \left(\exp\left[\frac{im}{2\hbar}\frac{(r_b - r_a)^2}{t_b - t_a}\right] - \exp\left[\frac{im}{2\hbar}\frac{(r_b + r_a)^2}{t_b - t_a}\right]\right)\end{aligned} \tag{2.89}$$

with $x_a = r_a$.

Chapter 3

Calculation and Results

3.1 Diffusion scenario

3.1.1 Barrier with known removal time

Consider a Brownian particle that starts on one side of a reflective wall located at $x = 0$. The wall is removed at $t = \Delta t_1$ and reinstated at $t = \Delta t_1 + \delta$. When the wall is removed, the particle can cross to the other side or stay. In this section, we will obtain the probability of finding the particle at some position at a time T. The one-dimensional free diffusion kernel is

$$K_F(x_0; x_N, \tau) = \left(\frac{1}{4\pi D\tau}\right)^{\frac{1}{2}} \exp\left[-\frac{(x_0 - x_N)^2}{4D\tau}\right], \tag{3.1}$$

the propagator for diffusion with a reflective wall is

$$K_W(x_0, x_N, \tau) = K_F(x_0; x_N, \tau) + K_F(x_0; -x_N, \tau), \tag{3.2}$$

which is obtained from solving the diffusion equation with initial condition

$$\lim_{\tau \to 0} K(x_0, x_N, \tau) = \delta(x_N - x_0), \tag{3.3}$$

and boundary condition

$$\lim_{x\to 0} \partial_x K(x_0, x, \tau) = 0. \tag{3.4}$$

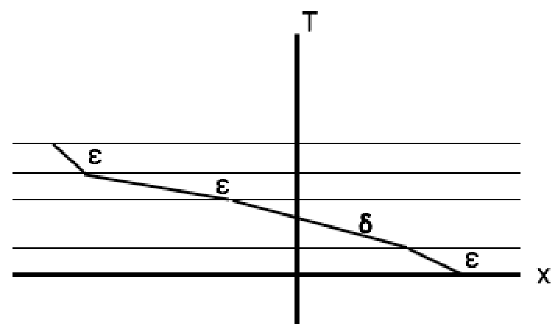


Figure 3.1: To compute the propagator, we divide the total time into $N-1$ segments of length ϵ and one segment of length δ; in this case, we have $N=4$ segments. The piece of length δ is a free particle propagator, while the others are wall propagators.

We will construct a path integral made of infinitesimal diffusion wall propagators (3.2), and change one of those by a free propagator (3.1). If the wall is located at $x=0$ and the particle starts at the positive side, all points before crossing will be integrated between $[0,\infty)$, and the points after crossing between $(-\infty,0]$. If the total time of the experiment is T, and the wall was removed for a time δ, then it was closed for a time $T-\delta$, we will divide the time it was closed in $N-1$ segments of length ϵ, so the total time will be $T=(N-1)\epsilon+\delta$, Figure 3.1 shows the time discretization when $N=4$. The propagator will be

$$\begin{aligned}
&\mathcal{K}_{A1}(x_0, x_N, \delta, \epsilon, k, N) = \\
&\left(\prod_{i=1}^{k}\int_0^\infty \mathrm{d}x_{i'}\right)\left(\prod_{j=k+1}^{N-1}\int_{-\infty}^0 \mathrm{d}x_j\right)\ \left(\prod_{i'=1}^{k} K_W(x_{i'-1}, x_{i'}, \epsilon)\right) K_F(x_k, x_{k+1}, \delta) \\
&\times\left(\prod_{j'=k+1}^{N-1} K_W(x_{j'}, x_{j'+1}, \epsilon)\right),
\end{aligned} \tag{3.5}$$

where the subscript A stands for "After", T is the total time, and $x_N \in (-\infty, 0]$. As the wall propagators satisfy the following Chapman-Kolmogorov equation for Markov processes [11]

$$\begin{aligned}\int_0^\infty \mathrm{d}x_1\ K_W(x_0,x_1,t_1-t_0)K_W(x_1,x_2,t_2-t_1) &= \int_{-\infty}^0 \mathrm{d}x_1\ K_W(x_0,x_1,t_1-t_0)K_W(x_1,x_2,t_2-t_1) \\ &= K_W(x_0,x_2,t_2-t_0), \end{aligned} \tag{3.6}$$

we end up with

$$\begin{aligned}&\mathcal{K}_{A1}(x_0,x_N,\delta,\epsilon,k,N) = \\ &\int_0^\infty \mathrm{d}x_k \int_{-\infty}^0 \mathrm{d}x_{k+1}\ K_W(x_0,x_k,k\epsilon)K_F(x_k,x_{k+1},\delta)K_W(x_{k+1},x_N,\epsilon(N-1-k)),\ \text{for } x_N<0\end{aligned} \tag{3.7}$$

Consider the case where the particle stays before the barrier instead of crossing within the time interval δ. The corresponding propagator is

$$\begin{aligned}&\mathcal{K}_{B1}(x_0,x_N,\delta,\epsilon,k,N) = \\ &\int_0^\infty \mathrm{d}x_k \int_0^\infty \mathrm{d}x_{k+1}\ K_W(x_0,x_k,k\epsilon)K_F(x_k,x_{k+1},\delta)K_W(x_{k+1},x_N,\epsilon(N-1-k)),\ \text{for } x_N>0\end{aligned} \tag{3.8}$$

where B stands for "Before". Adding this together, the total propagator will be

$$K_1(x_0,x_N,\delta,\epsilon,k,N) = \mathcal{K}_{B1}(x_0,x_N,\delta,\epsilon,k,N)\Theta(x_N) + \mathcal{K}_{A1}(x_0,x_N,\delta,\epsilon,k,N)\Theta(-x_N). \tag{3.9}$$

The integrals in equations (3.7), (3.8) are solved analytically, yet the explicit expression is not shown here since it is rather complicated (see Appendix B). Figure 3.2 shows equation (3.9) as a function of x_N for different δ, here we use the constraint $\epsilon = \frac{T-\delta}{N-1}$ that states that for a fixed total time T and partition N, the time steps ϵ have to vary as a function of δ. We observe that when $\delta \to T$, the curve approaches the free particle, and conversely, when $\delta \to 0$, the curve tends to the reflective wall. This is a direct consequence of the

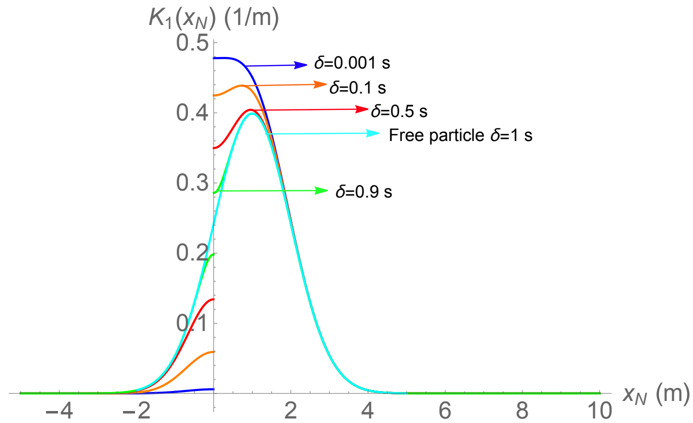


Figure 3.2: Probability density K_1 as a function of the position x_N given that the particle starts at $x_0 = 1$ m, with a diffusion coefficient $d = 0.5$ m^2 s^{-1}, a total time $T = 1$ sec, a crossing step $k = 2$ and a partition $N = 5$. The different curves are for $\delta = 0.001, 0.1, 0.5, 0.9$ and 1 sec.

propagator's construction: setting $\delta = 0$ in equations (3.7), (3.8) we obtain

$$\mathcal{K}_{B1}(x_0, x_N, \delta, \epsilon, k, N) =$$
$$\int_0^\infty \mathrm{d}x_k \int_0^\infty \mathrm{d}x_{k+1}\ K_W(x_0, x_k, k\epsilon)\delta(x_k - x_{k+1})K_W(x_{k+1}, x_N, \epsilon(N-1-k)),\ \text{for } x_N > 0$$
$$\mathcal{K}_{A1}(x_0, x_N, \delta, \epsilon, k, N) =$$
$$\int_0^\infty \mathrm{d}x_k \int_{-\infty}^0 \mathrm{d}x_{k+1}\ K_W(x_0, x_k, k\epsilon)\delta(x_k - x_{k+1})K_W(x_{k+1}, x_N, \epsilon(N-1-k)),\ \text{for } x_N < 0$$

where $\delta(x_k, x_{k+1})$ is the Dirac delta. Solving the x_{k+1} integral for $\mathcal{K}_{B1}$ we get

$$\begin{aligned}\mathcal{K}_{B1}(x_0, x_N, \delta, \epsilon, k, N) &= \int_0^\infty \mathrm{d}x_k\ K_W(x_0, x_k, k\epsilon)K_W(x_k, x_N, \epsilon(N-1-k)) \\ &= K_W(x_0, x_N, \epsilon(N-1)),\ \text{for } x_N > 0.\end{aligned}$$

and using $T = (N-1)\epsilon + \delta = (N-1)\epsilon$, $\mathcal{K}_{B1}$ becomes

$$\mathcal{K}_{B1} = K_W(x_0, x_N, T),\ \text{for } x_N > 0,\ \delta = 0. \tag{3.10}$$

In the case of $\mathcal{K}_{A1}$, since $x_k > 0$ and $x_{k+1} < 0$, the integration of the Dirac delta gives zero, thus $\mathcal{K}_{A1}$ for $\delta = 0$. Therefore, the total propagator for $\delta = 0$ is

$$K_1(x_0, x_N, T) = K_{A1}(x_0, x_N, T)\Theta(-x_N) + K_{B1}(x_0, x_N, T)\Theta(x_N) = K_W(x_0, x_N, T)\Theta(x_N) \tag{3.11}$$

Now, for $\delta = T$ we have $\epsilon = \frac{T-\delta}{N-1} = 0$, so the two wall propagators of equations (3.7), (3.8) will become Dirac deltas, giving

$$\mathcal{K}_{B1}(x_0, x_N, T) = \int_0^\infty \mathrm{d}x_k \int_0^\infty \mathrm{d}x_{k+1}\ \delta(x_0, x_k) K_F(x_k, x_{k+1}, T)\delta(x_{k+1}, x_N),\ \text{for } x_N > 0$$

$$\mathcal{K}_{A1}(x_0, x_N, T) = \int_0^\infty \mathrm{d}x_k \int_{-\infty}^0 \mathrm{d}x_{k+1}\ \delta(x_0, x_k) K_F(x_k, x_{k+1}, T)\delta(x_{k+1}, x_N),\ \text{for } x_N < 0.$$

Solving the integrals we have

$$\begin{aligned} \mathcal{K}_{B1}(x_0, x_N, T) &= K_F(x_0, x_N, T),\ \text{for } x_N > 0 \\ \mathcal{K}_{A1}(x_0, x_N, T) &= K_F(x_0, x_N, T),\ \text{for } x_N < 0, \end{aligned} \tag{3.12}$$

arriving to the free propagator as expected

$$K_1(x_0, x_N, T) = K_F(x_0, x_N, T)\Theta(x_N) + K_F(x_0, x_N, T)\Theta(-x_N) = K_F(x_0, x_N, T) \tag{3.13}$$

From Figure 3.2, we observe a discontinuity at $x = 0$, meaning that the propagator for the left side has a different value at the boundary than the one from the right. In the reflective wall the probability density drops abruptly to zero at the boundary, and conversely, in the free particle case there is no discontinuity at all. Being an interpolation between those two cases, our propagator K_1 shows a gap at $x = 0$ that decreases as $\delta \to T$ (Figure 3.2). Further, we can obtain the explicit value of that gap via

$$\Delta K_1 = \mathcal{K}_{B1}(x_0, x_N, \delta, \epsilon, k, N) - \mathcal{K}_{A1}(x_0, x_N, \delta, \epsilon, k, N)\Big|_{x_N=0} \tag{3.14}$$

which, using the explicit values of $\mathcal{K}_{B1}$ and $\mathcal{K}_{A1}$ from eqs. (B.8) & (B.9) is

$$\Delta K_1 = \frac{e^{-\frac{x_0^2}{4D(\delta+\epsilon(-k+N-1)+k\epsilon)}}}{\sqrt{\pi D(\delta+\epsilon(-k+N-1)+k\epsilon)}}\left(1-4T\left(\alpha,\beta\right)\right) \tag{3.15}$$

where $T(\alpha,\beta)$ is the Owen's T function [30] and

$$\alpha \equiv \frac{x_0\sqrt{\epsilon(-k+N-1)}}{\sqrt{2D(\delta+k\epsilon)(\delta+\epsilon(-k+N-1)+k\epsilon)}}$$
$$\beta \equiv \frac{\sqrt{\delta(\delta+\epsilon(-k+N-1)+k\epsilon)}}{\epsilon\sqrt{k(-k+N-1)}}.$$

Note that when δ is zero, β becomes zero too and the Owen's T function vanishes, giving

$$\Delta K_1 = \frac{e^{-\frac{x_0^2}{4D\epsilon(+N-1)}}}{\sqrt{\pi D\epsilon(N-1)}} = \frac{e^{-\frac{x_0^2}{4DT}}}{\sqrt{\pi DT}} \tag{3.16}$$

which is precisely the reflecting wall propagator (3.2) evaluated at $x_N = 0$.
Conversely, if δ is the total time T, then ϵ is zero; causing α to vanish and β to be infinitely large. The Owen's function becomes

$$\lim_{\beta\to\infty} T(0,\beta) = \frac{1}{4},$$

thus giving $\Delta K_1 = 0$, which is the free particle case.
Figure 3.3 shows ΔK_1 from equation (3.15) as a function of δ. Four curves are plotted, each for a different total time T; here we see the interpolation from the reflecting wall to the free particle obtained above. Next is to show that the total probability is normalized to one, i.e

$$\int_0^\infty \mathrm{d}x_N\ \mathcal{K}_{B1}(x_0,x_N,\delta,\epsilon,k,N) + \int_{-\infty}^0 \mathrm{d}x_N\ \mathcal{K}_{A1}(x_0,x_N,\delta,\epsilon,k,N) = 1. \tag{3.17}$$

The proof goes as follows: let P_{B1} and P_{A1} be the probabilities for the particle to be before or after the barrier, respectively. Since the integrand is a squared integrable

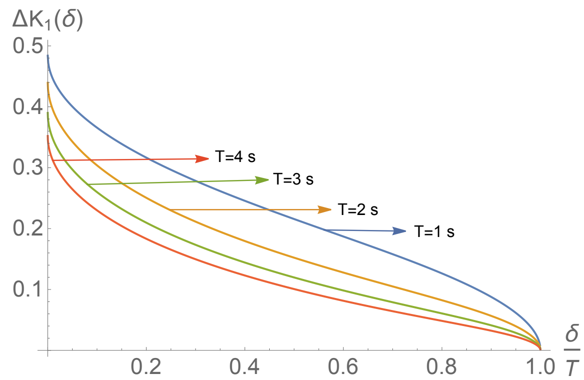


Figure 3.3: Equation (3.15) is plotted as a function of δ, each curve is for a different total time T. We used a diffusion coefficient of $D = 0.5$ m^2 s^{-1}, initial position $x_0 = 1$ m, crossing step $k = 2$ and a partition $N = 5$

function, we can swap the integrals to get

$$\begin{aligned}P_{A1}(x_0,T) &= \int_{-\infty}^{0} \mathrm{d}x_N \int_{0}^{\infty} \mathrm{d}x_1 \int_{-\infty}^{0} \mathrm{d}x_2\; K_W(x_0,x_1,\Delta t_1)K_F(x_1,x_2,\delta)K_W(x_2,x_N,T-\delta-\Delta t_1)\\ &= \int_{0}^{\infty} \mathrm{d}x_1 \int_{-\infty}^{0} \mathrm{d}x_2 \int_{-\infty}^{0} \mathrm{d}x_N\; K_W(x_0,x_1,\Delta t_1)K_F(x_1,x_2,\delta)K_W(x_2,x_N,T-\delta-\Delta t_1),\end{aligned} \tag{3.18}$$

defining $\Delta t_2 = T - \delta - \Delta t_1$ we have that (3.18) is

$$\begin{aligned}&P_{A1} =\\ &\left(\frac{1}{4\pi D\Delta t_1}\right)^{\frac{1}{2}}\left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}}\left(\frac{1}{4\pi D\Delta t_2}\right)^{\frac{1}{2}}\int_0^\infty \mathrm{d}x_1\int_{-\infty}^0 \mathrm{d}x_2\int_{-\infty}^0 \mathrm{d}x_N \left(e^{-\frac{(x_0-x_1)^2}{4D\Delta t_1}}+e^{-\frac{(x_0+x_1)^2}{4D\Delta t_1}}\right)e^{-\frac{(x_1-x_2)^2}{4D\delta}}\\ &\times\left(e^{-\frac{(x_2-x_N)^2}{4D\Delta t_2}}+e^{-\frac{(x_2+x_N)^2}{4D\Delta t_2}}\right)\\ &=\left(\frac{1}{4\pi D\Delta t_1}\right)^{\frac{1}{2}}\left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}}\int_0^\infty \mathrm{d}x_1\int_{-\infty}^0 \mathrm{d}x_2\; e^{-\frac{(x_1-x_2)^2}{4D\delta}}\left(e^{-\frac{(x_1-x_0)^2}{4D\Delta t_1}}+e^{-\frac{(x_1+x_0)^2}{4D\Delta t_1}}\right)\end{aligned} \tag{3.19}$$

Analogously for the right side

$$P_{B1} = \left(\frac{1}{4\pi D\Delta t_1}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \int_0^\infty \mathrm{d}x_1 \int_0^\infty \mathrm{d}x_2 \; e^{-\frac{(x_1-x_2)^2}{4D\delta}} \left(e^{-\frac{(x_1-x_0)^2}{4D\Delta t_1}} + e^{-\frac{(x_1+x_0)^2}{4D\Delta t_1}}\right) \tag{3.20}$$

We can sum up the integrals over $\mathrm{d}x_2$ to obtain

$$P_{A1} + P_{B1} = \left(\frac{1}{4\pi D\Delta t_1}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^\infty \mathrm{d}x_2 \; e^{-\frac{(x_1-x_2)^2}{4D\delta}} \left(e^{-\frac{(x_1-x_0)^2}{4D\Delta t_1}} + e^{-\frac{(x_1+x_0)^2}{4D\Delta t_1}}\right), \tag{3.21}$$

and solving the integrals we find

$$P_{A1} + P_{B1} = 1. \tag{3.22}$$

These probabilities can be expressed in terms of the the Owen's T function $T(a,b)$ [30].

$$P_{A1}(x_0, D, \delta, \Delta t_1) = 2T\left(x_0\sqrt{\frac{1}{2D(\delta+\Delta t_1)}}, \sqrt{\frac{\delta}{\Delta t_1}}\right) \tag{3.23}$$

$$P_{B1}(x_0, D, \delta, \Delta t_1) = \left(1 - 2T\left(x_0\sqrt{\frac{1}{2D(\delta+\Delta t_1)}}, \sqrt{\frac{\delta}{\Delta t_1}}\right)\right). \tag{3.24}$$

On the other hand, if $\delta \ll \Delta t_1$ we can Taylor-expand the Owen's T function as follows

$$T(\alpha, \beta) \approx \frac{e^{-\frac{\alpha^2}{2}}\beta}{2\pi} + O(\beta^3)\ ,\ \text{for } \beta \ll 1 \tag{3.25}$$

with $\beta = \sqrt{\frac{\delta}{\Delta t_1}}$, we obtain

$$P_A \approx \frac{\sqrt{\delta}}{\pi\sqrt{\Delta t_1}} e^{-\frac{x_0^2}{4D\Delta t_1}}. \tag{3.26}$$

The probability for the particle to be after the wall is $O(\delta^{1/2})$ for $\delta \ll \Delta t_1$.

3.1.2 Barrier with unknown removal time: The demon.

Now consider a reflecting boundary at $x = 0$ that is guarded by a "demon" who can remove it **once** at a time between $[0, T]$, for a time δ. As in the previous case, the Brownian particle is initially at $x = x_0$ and crosses from the ray $[0, \infty)$ to $(-\infty, 0]$. Since the barrier opens at a time between $t = \epsilon$ and $t = (N-2)\epsilon$, we obtain the propagator by summing over all possible $t_k = k\epsilon$ within $k = [1, N-2]$.

$$\begin{aligned}\mathcal{K}_{A2}(x_N, x_0, D, \delta, \epsilon, N) =& A\left(\frac{m}{4\pi D\epsilon}\right)^{\frac{N-1}{2}} \left(\frac{m}{4\pi D\delta}\right)^{\frac{1}{2}} \sum_{k=1}^{N-2} \left(\prod_{i'=k+1}^{N-1} \int_{-\infty}^{0} \mathrm{d}x_{i'}\right) \left(\prod_{i=1}^{k} \int_{0}^{\infty} \mathrm{d}x_i\right) \\ &\times \left(\prod_{j=1}^{k} K_W(x_{j-1}, x_j, \epsilon)\right) K_F(x_k, x_{k+1}, \delta) \\ &\times \left(\prod_{j'=k+1}^{N-1} K_W(x_{j'}, x_{j'+1}, T - k\epsilon - \delta)\right), \end{aligned} \tag{3.27}$$

where the subscript A stands for "After" since this propagator describes the probability density after crossing the barrier, $T = (N-1)\epsilon + \delta$ and A is a normalization constant. As the wall propagators satisfy the following Chapman-Kolmogorov equation (3.6), we write

$$\begin{aligned}&\mathcal{K}_{A2}(x_N, x_0, D, \delta, \epsilon, N) = \\ &A \sum_{k=1}^{N-2} \left(\frac{1}{4\pi Dk\epsilon}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\Delta t_2}\right)^{\frac{1}{2}} \int_{0}^{\infty} \mathrm{d}x_k \int_{-\infty}^{0} \mathrm{d}x_{k+1} \left(e^{-\frac{(x_0-x_k)^2}{4Dk\epsilon}} + e^{-\frac{(x_0+x_k)^2}{4Dk\epsilon}}\right) e^{-\frac{(x_k-x_{k+1})^2}{4D\delta}} \\ &\times \left(e^{-\frac{(x_{k+1}-x_N)^2}{4D\Delta t_2}} + e^{-\frac{(x_{k+1}+x_N)^2}{4D\Delta t_2}}\right). \end{aligned} \tag{3.28}$$

where $\Delta t_2 = T - k\epsilon - \delta$. As in the previous case, we compute the probability density to find a particle before the boundary (i.e., on the positive half-plane) at time $T = (N-1)\epsilon + \delta$. This propagator is very similar to (3.28), only with a change in the integration limits of the x_{k+1} integral

$$\mathcal{K}_{B2}(x_N, x_0, D, \delta, \epsilon, N) =$$
$$A \sum_{k=1}^{N-2} \left(\frac{1}{4\pi D k\epsilon}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\Delta t_2}\right)^{\frac{1}{2}} \int_0^\infty \mathrm{d}x_k \int_0^\infty \mathrm{d}x_{k+1} \left(e^{-\frac{(x_0-x_k)^2}{4Dk\epsilon}} + e^{-\frac{(x_0+x_k)^2}{4Dk\epsilon}}\right) e^{-\frac{(x_k-x_{k+1})^2}{4D\delta}}$$
$$\times \left(e^{-\frac{(x_{k+1}-x_N)^2}{4D\Delta t_2}} + e^{-\frac{(x_{k+1}+x_N)^2}{4D\Delta t_2}}\right). \tag{3.29}$$

Plugging this together, we obtain the total probability density

$$K_2(x_N, x_0, D, \delta, \epsilon, N) = \mathcal{K}_{B2}(x_N, x_0, D, \delta, \epsilon, N)\Theta(x_N) + \mathcal{K}_{A2}(x_N, x_0, D, \delta, \epsilon, N)\Theta(-x_N). \tag{3.30}$$

Now we proceed to find the normalization factor needed to fulfill the condition

$$\int_{-\infty}^0 \mathrm{d}x_N\ \mathcal{K}_{A2}(x_N, x_0, D, \delta, \epsilon, N) + \int_0^\infty \mathrm{d}x_N\ \mathcal{K}_{B2}(x_N, x_0, D, \delta, \epsilon, N) = 1. \tag{3.31}$$

Define

$$P_{A2}(x_0, D, \delta, \epsilon, N) = \int_{-\infty}^0 \mathrm{d}x_N\ K_{A2}(x_N, x_0, D, \delta, \epsilon, N) \tag{3.32}$$
$$P_{B2}(x_0, D, \delta, \epsilon, N) = \int_0^\infty \mathrm{d}x_N\ \mathcal{K}_{B2}(x_N, x_0, D, \delta, \epsilon, N), \tag{3.33}$$

we have

$$P_{A2}(x_0, D, \delta, \epsilon, N) =$$
$$A \int_{-\infty}^0 \mathrm{d}x_N \sum_{k=1}^{N-2} \left(\frac{1}{4\pi D\Delta t_1}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\Delta t_2}\right)^{\frac{1}{2}} \int_0^\infty dx_k \int_{-\infty}^0 dx_{k+1} \left(e^{-\frac{(x_0-x_k)^2}{4D\Delta t_1}} + e^{-\frac{(x_0+x_k)^2}{4D\Delta t_1}}\right)$$
$$\times e^{-\frac{(x_k-x_{k+1})^2}{4D\delta}} \left(e^{-\frac{(x_{k+1}-x_N)^2}{4D\Delta t_2}} + e^{-\frac{(x_{k+1}+x_N)^2}{4D\Delta t_2}}\right). \tag{3.34}$$

Entering the x_N integral in the sum and following the same procedure as in sec. 3.1.1

we find

$$P_{A2}(x_0, D, \delta, \epsilon, N) =$$
$$A \sum_{k=1}^{N-2} \left(\frac{1}{4\pi D \Delta t_1}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D \delta}\right)^{\frac{1}{2}} \int_0^\infty dx_k \int_{-\infty}^0 dx_{k+1}\, e^{-\frac{(x_k - x_{k+1})^2}{4D\delta}} \left(e^{-\frac{(x_k - x_0)^2}{4D\Delta t_1}} + e^{-\frac{(x_k + x_0)^2}{4D\Delta t_1}}\right), \tag{3.35}$$

analogously for the right side

$$P_{B2}(x_0, D, \delta, \epsilon, N) =$$
$$A \sum_{k=1}^{N-2} \left(\frac{1}{4\pi D \Delta t_1}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D \delta}\right)^{\frac{1}{2}} \int_0^\infty dx_k \int_0^\infty dx_{k+1}\, e^{-\frac{(x_k - x_{k+1})^2}{4D\delta}} \left(e^{-\frac{(x_k - x_0)^2}{4D\Delta t_1}} + e^{-\frac{(x_k + x_0)^2}{4D\Delta t_1}}\right). \tag{3.36}$$

Carrying out the integrals and the sum we finally have

$$P_{A2}(x_0, D, \delta, \epsilon, N) + P_{B2}(x_0, D, \delta, \epsilon, N) = A(N-2) = 1, \tag{3.37}$$

then

$$A = \frac{1}{N-2} \tag{3.38}$$

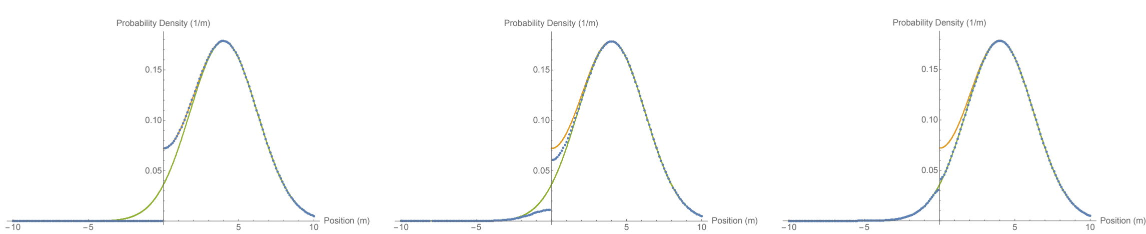


Figure 3.4: Probability density at $T = 5$ sec. for a Brownian particle that starts at $x_0 = 4$ m given that: (1) is in the presence of a reflective wall (orange), (2) is in the presence of a demon (blue points), (3) is free (green). The three different plots account for $\delta = 0.0001, 2.5, 4.9$ sec. respectively. We consider a partition of $N = 4$.

Figure 3.4 shows a comparison between the probability densities of the free particle, the reflecting wall, and the wall with a demon. We note that when $\delta \to 0$, the wall with a demon approaches the reflective wall (left plot), and conversely, when $\delta \to T = 5$ sec, it approaches the free particle (right plot). The latter we stated in the previous section is a consequence of the propagator's construction. The middle plot shows neither full reflective nor total free propagation, but a wall with a demon that removes it for a time $\delta = \frac{T}{2} = 2.5$ sec.

Going back to the total probabilities, we have

$$P_{A2}(x_0, D, \delta, \epsilon, N) = \left(\frac{1}{N-2}\right) \sum_{k=1}^{N-2} \left(\frac{1}{4\pi D k\epsilon}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \int_0^{\infty} dx_k \int_{-\infty}^{0} dx_{k+1}\ e^{-\frac{(x_k - x_{k+1})^2}{4D\delta}} \times \left(e^{-\frac{(x_k - x_0)^2}{4Dk\epsilon}} + e^{-\frac{(x_k + x_0)^2}{4Dk\epsilon}}\right), \tag{3.39}$$

$$P_{B2}(x_0, D, \delta, \epsilon, N) = \left(\frac{1}{N-2}\right) \sum_{k=1}^{N-2} \left(\frac{1}{4\pi D k\epsilon}\right)^{\frac{1}{2}} \left(\frac{1}{4\pi D\delta}\right)^{\frac{1}{2}} \int_0^{\infty} dx_k \int_{0}^{\infty} dx_{k+1}\ e^{-\frac{(x_k - x_{k+1})^2}{4D\delta}} \times \left(e^{-\frac{(x_k - x_0)^2}{4Dk\epsilon}} + e^{-\frac{(x_k + x_0)^2}{4Dk\epsilon}}\right). \tag{3.40}$$

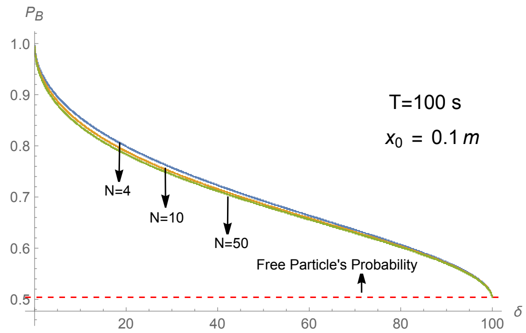
which can be expressed in terms of the the Owen's T function $T(a, b)$ [30] as follows

$$P_{A2}(x_0, D, \delta, \epsilon, N) = \frac{1}{N-2} \sum_{k=1}^{N-2} 2T\left(x_0\sqrt{\frac{1}{2D(\delta + k\epsilon)}}, \sqrt{\frac{\delta}{k\epsilon}}\right) \tag{3.41}$$

$$P_{B2}(x_0, D, \delta, \epsilon, N) = \frac{1}{N-2} \sum_{k=1}^{N-2} \left(1 - 2T\left(x_0\sqrt{\frac{1}{2D(\delta + k\epsilon)}}, \sqrt{\frac{\delta}{k\epsilon}}\right)\right). \tag{3.42}$$

Figure 3.5 shows equations (3.41), (3.42) as a function of the opening time δ for different partitions N. To impose a fixed total time T we set $\epsilon = \frac{T-\delta}{N-1}$, so that when δ increases, the time slice ϵ decreases. We note that as $\delta \to 0$ the probability before the barrier approaches one and after the barrier approaches zero. On the other hand, if $\delta \to T$ both probabilities approach the free particle case, which is the expected result. In conclusion, the smaller parameter δ, the more confident we are that the particle is before the barrier.

A rigorous way to measure how certain we are of an outcome in a probabilistic experiment is the Shannon's entropy. Given an experiment of two possible outcomes, one of them with



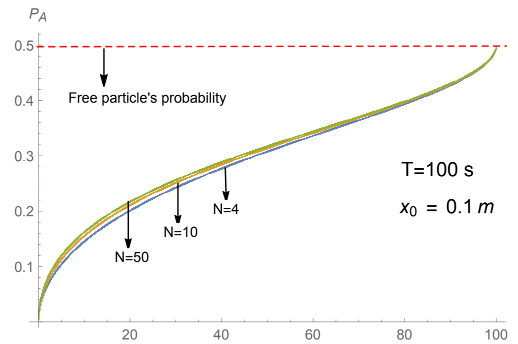


Figure 3.5: Probability of a Brownian particle that starts at $x_0 = 0.1$ m to be measured at $T = 100$ s before (P_B) or after (P_A) the barrier when it is removed for a time δ s at any moment. Three curves, one for each $N = 4, 10, 50$ are shown. In dashed line is the probability to find a free particle at $T = 100$ s released at the same point.

probability p, the Shannon's entropy reads

$$H(p) = -p\log(p) - (1-p)\log(1-p). \tag{3.43}$$

If we use our probabilities P_A and $P_B = 1 - P_A$, we can obtain the entropy as a function of δ as shown in Figure 3.6. If $\delta = 0$ then $P_B = 1$ which leads to $H = 0$ according to (3.43),

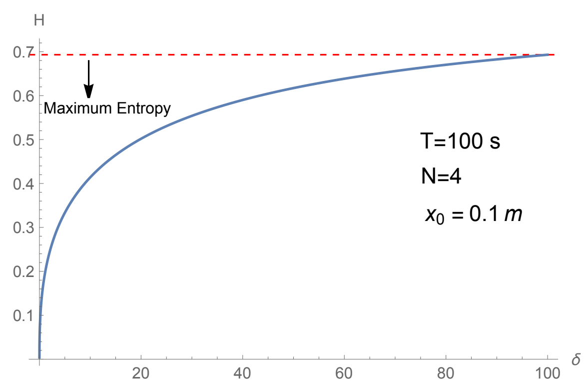


Figure 3.6: Shannon entropy as a function of δ for fixed values of total time $T = 100$ s, partition $N = 4$, and initial position $x_0 = 0.1$ m.

in this case we know for certain that the particle has not crossed the boundary, fact that minimizes the entropy. The probability for a free particle to be after the barrier is

$$P_0(D, x_0, T) = \frac{1}{2}\mathrm{erfc}\left(\frac{1}{2}x_0\sqrt{\frac{1}{DT}}\right), \tag{3.44}$$

we note that it approaches $\frac{1}{2}$ when T is large. Also, note that the entropy (3.43) has a maximum at $p = \frac{1}{2}$, thus, the free particle reaches maximum entropy at long times. For $T = 100$ s, $d = 0.5$ m^{2}s^{-1}, $x_0 = 0.1$ m, we have that $P_0 = 0.496$ and the entropy is almost maximal. In particular, our system reaches its maximum entropy when it tends to the free particle ($\delta \to T$) as shown in Figure 3.6.

Further, we can study the dependence of the propagator on the time partition N. Figure 3.7 shows the configurations considered when computing the total probability for $N = 5$, recall that the demon can open the barrier right after the first (wall) propagator until right before the last, so if $N = 5$ there are three possibilities. In general there are $N - 2$ configurations we add together to obtain the total probability.

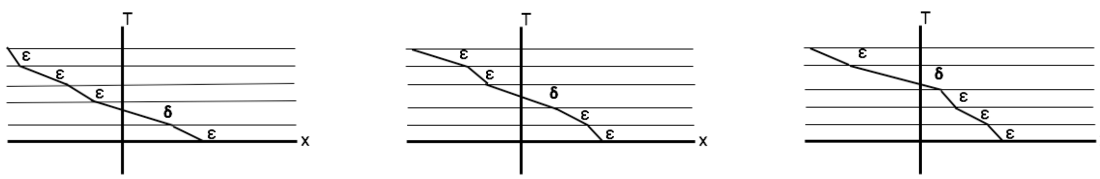


Figure 3.7: Possible configurations that sum up the Brownian particle's total probability to cross to the other side if we divide the time into N=5 segments. When the barrier is closed, the segments are of length ϵ and δ when it is open.

Figure 3.8 shows the probability density (3.30) for different N. We find that the curve changes very slowly, and mainly at the boundary, an increase in N results in a decrease of the probability density at the boundary before crossing, and an increase after crossing. If

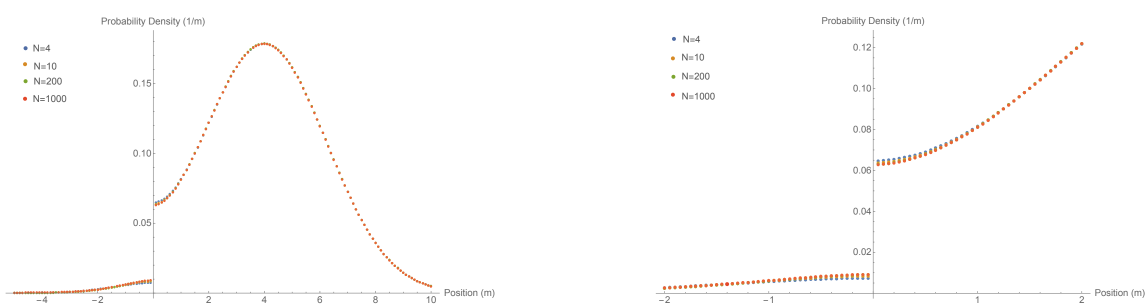
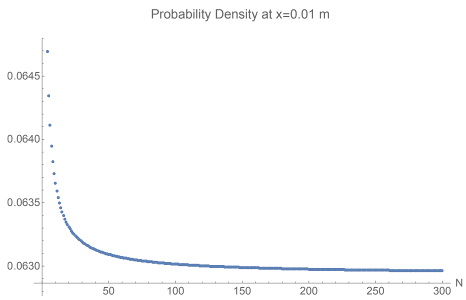


Figure 3.8: Probability density for the barrier with demon as a function of the position for different partitions $N = 4, 10, 200, 1000$. The right plot is a close-up of the left plot at the boundary.

we were to take the limit $N \to \infty$, which is the exact path integral, it seems to converge to a finite value. To reinforce this affirmation, we take a point near the boundary from the curve 3.8 and plot it as a function of N (Figure 3.9). We observe that indeed for large N, the curve saturates to a constant value.



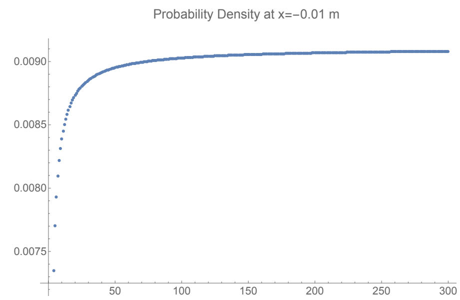


Figure 3.9: Probability density at $x = 0.01$ m (left) and $x = -0.01$ m (right) for the barrier with demon as a function of the number of partitions N.

3.2 Quantum scenario

3.2.1 Barrier with known removal time

This section addresses the case of a quantum particle in the presence of a reflective wall potential that is turned off and on at known times. The procedure follows in the same fashion as the diffusion case in section 3.1.1. However, the reader does not need knowledge of the previous sections.

Consider a reflecting wall located at $x = 0$ and a quantum particle that is initially at $x_0 > 0$, the wall is removed at $t = \Delta t_1$ and reinstated at $t = \Delta t_1 + \delta$. When the wall is removed, the particle can either cross to the other side or stay. We aim to obtain the probability of finding the particle at some position at a time T given that the wall is removed for a time δ. In Chapter 2 we obtained that the one-dimensional Schrodinger propagator is

$$K_0(x_0, x_N, T) = \sqrt{\frac{m}{2\pi i\hbar T}} \exp\left[\frac{im}{2\hbar T}(x_0 - x_N)^2\right], \tag{3.45}$$

and for a particle in the presence of a reflecting wall at $x = 0$ the propagator becomes

$$K_W(x_0, x_N, T) = K_0(x_0; x_N, T) - K_0(x_0; -x_N, T). \tag{3.46}$$

We construct a path integral made of infinitesimal half space propagators (3.46), and change one of those by a free propagator (3.45). If the total time of the experiment is T, and the wall was opened for a time δ, then it was closed for a time $T-\delta$, we divide the time it was closed in $N-1$ segments of length ϵ; thus the total time will be $T=(N-1)\epsilon+\delta$. Figure 3.1 shows the time discretization when $N=4$. Let $\mathcal{K}_{Aqm}$ be the probability amplitude that the particle is at $x_N<0$ after a time T given that started at $x_0>0$, then

$$\begin{aligned}
&\mathcal{K}_{Aqm}(x_0,x_N,T) = \\
&\left(\prod_{i=1}^{k}\int_0^\infty \mathrm{d}x_{i'}\right)\left(\prod_{j=k+1}^{N-1}\int_{-\infty}^0 \mathrm{d}x_j\right)\ \left(\prod_{i'=1}^{k} K_W(x_{i'-1},x_{i'},\epsilon)\right) K_0(x_k,x_{k+1},\delta) \\
&\times\left(\prod_{j'=k+1}^{N-1} K_W(x_{j'},x_{j'+1},\epsilon)\right),
\end{aligned} \tag{3.47}$$

where $k\in[1,N-2]$ is the crossing step, and the subscript A stands for "After" the barrier. As the wall propagators satisfy the following Chapman-Kolmogorov equation (3.6), we obtain

$$\mathcal{K}_{Aqm}(x_0,x_N,\Delta t_1,\delta,\Delta t_2) = \int_0^\infty \mathrm{d}x_1\int_{-\infty}^0 \mathrm{d}x_2\ K_W(x_0,x_1,\Delta t_1)K_0(x_1,x_2,\delta)K_W(x_2,x_N,\Delta t_2). \tag{3.48}$$

where $\Delta t_1+\delta+\Delta t_2=T$. Similarly, the probability amplitude that the particle is at $x_N>0$ after a time T given that started at $x_0>0$ is

$$\mathcal{K}_{Bqm}(x_0,x_N,\Delta t_1,\delta,\Delta t_2) = \int_0^\infty \mathrm{d}x_1\int_0^\infty \mathrm{d}x_2\ K_W(x_0,x_1,\Delta t_1)K_0(x_1,x_2,\delta)K_W(x_2,x_N,\Delta t_2). \tag{3.49}$$

where B stands for "Before" the barrier. If we take an arbitrary normalized initial state $\psi_0(x_0)$, the corresponding wave functions will be

$$\begin{aligned}\psi_A(x,\delta,\Delta t_1,\Delta t_2) &= \int \mathrm{d}x_0\ \psi_0(x_0)\mathcal{K}_{Aqm}(x_0,x,\Delta t_1,\delta,T)\\ &= \int \mathrm{d}x_0\ \psi_0(x_0)\int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2\ K_W(x_0,x_1,\Delta t_1)K_0(x_1,x_2,\delta)K_W(x_2,x,\Delta t_2).\end{aligned} \tag{3.50}$$

$$\begin{aligned}\psi_B(x,\delta,\Delta t_1,\Delta t_2) &= \int \mathrm{d}x_0\ \psi_0(x_0)\mathcal{K}_{Bqm}(x_0,x,\Delta t_1,\delta,T)\\ &= \int \mathrm{d}x_0\ \psi_0(x_0)\int_0^\infty \mathrm{d}x_1 \int_0^\infty \mathrm{d}x_2\ K_W(x_0,x_1,\Delta t_1)K_0(x_1,x_2,\delta)K_W(x_2,x,\Delta t_2),\end{aligned} \tag{3.51}$$

and the total wave function is

$$\psi(x,\delta,\Delta t_1,\Delta t_2) = \psi_A(x,\delta,\Delta t_1,\Delta t_2)\Theta(-x) + \psi_B(x,\delta,\Delta t_1,\Delta t_2)\Theta(x). \tag{3.52}$$

Thus, the probability is given by

$$\begin{aligned}\int_{-\infty}^\infty \mathrm{d}x\ |\psi(x,\delta,\Delta t_1,\Delta t_2)|^2 &= \int_{-\infty}^\infty \mathrm{d}x\ |\psi_A(x,\delta,\Delta t_1,\Delta t_2)\Theta(-x) + \psi_B(x,\delta,\Delta t_1,\Delta t_2)\Theta(x)|^2\\ &= \int_{-\infty}^0 \mathrm{d}x|\psi_A(x,\delta,\Delta t_1,\Delta t_2)|^2 + \int_0^\infty \mathrm{d}x|\psi_B(x,\delta,\Delta t_1,\Delta t_2)|^2.\end{aligned} \tag{3.53}$$

First, note that both ψ_A, ψ_B satisfy the Schrödinger equation with respect to Δt_2. For ψ_A we have

$$\begin{aligned} i\hbar\frac{\mathrm{d}\psi_A}{\mathrm{d}\Delta t_2} &= \int \mathrm{d}x_0\ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2\ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x_2, \delta) i\hbar \frac{\mathrm{d}K_W(x_2, x, \Delta t_2)}{\mathrm{d}\Delta t_2} \\ &= \int \mathrm{d}x_0\ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2\ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x_2, \delta) \left(-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2 K_W(x_2, x, \Delta t_2)}{\mathrm{d}x^2} \right) \\ &= -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \int \mathrm{d}x_0\ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2\ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x_2, \delta) K_W(x_2, x, \Delta t_2) \\ &= -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_A}{\mathrm{d}x^2}, \end{aligned} \tag{3.54}$$

which implies that the probability

$$P_A = \int_{-\infty}^0 \mathrm{d}x\ |\psi_A|^2 \tag{3.55}$$

does not change with Δt_2 provided that $|\psi_A(x \to -\infty)| = |\psi_A(x \to 0)| = 0$ (Appendix C). An analogous procedure can be carried out to conclude the same for ψ_B. Given that $\int_{-\infty}^0 \mathrm{d}x\ |\psi_A|^2$ and $\int_0^\infty \mathrm{d}x\ |\psi_B|^2$ do not change with Δt_2, we can study these probabilities at $\Delta t_2 = 0$ to simplify the computation. Using the property $K_W(x_2, x; \Delta t_2 = 0) = \delta(x_2 - x)$, we have

$$\psi_A(x, \delta, \Delta t_1, \Delta t_2 = 0) = \int \mathrm{d}x_0\ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2\ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x_2, \delta) \delta(x_2 - x), \tag{3.56}$$

which leads to

$$\psi_A(x, \delta, \Delta t_1, \Delta t_2 = 0) = \int \mathrm{d}x_0\ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1\ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x, \delta),\ \text{for } x < 0 \tag{3.57}$$

Similarly for ψ_B we have

$$\psi_B(x, \delta, \Delta t_1, \Delta t_2 = 0) = \int \mathrm{d}x_0 \ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1 \ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x, \delta), \ \text{for } x > 0 \tag{3.58}$$

thus, the total wave function at $\Delta t_2 = 0$ is

$$\psi(x, \delta, \Delta t_1, 0) = \int \mathrm{d}x_0 \ \psi_0(x_0) \int_0^\infty \mathrm{d}x_1 \ K_W(x_0, x_1, \Delta t_1) K_0(x_1, x, \delta), \ \text{for all } x \tag{3.59}$$

If we also set $\Delta t_1 = 0$, the wave function (3.59) becomes

$$\psi(x, \delta, 0, 0) = \int \mathrm{d}x_0 \ \psi_0(x_0) K_0(x_0, x, \delta), \ \text{for all } x, \tag{3.60}$$

this case was already studied by Marchweka & Schuss [22] considering an initial wave function with compact support. They conclude that the probability propagated across the wall is $O(\delta^{3/2})$ which recovers the Zeno effect for continuous detection of a particle in a given domain [23]. A more in-depth study of the wave function (3.52) and its applications will be left for future work.

Chapter 4

Summary and Conclusions

This work aims to describe a barrier that is neither purely absorbing nor purely reflecting, but a reflecting barrier removed and reinstated. We first consider the case of a Brownian particle that starts on one side of a reflective barrier which is removed once at $t = \Delta t_1$ and reinstated at $t = \Delta t_1 + \delta$. The construction is such that when δ tends to zero, we recover the known probability density of a reflective wall, and when this time tends to the total time, we recover free particle's probability density. We obtained the path-integral propagator and a closed expression for the particle's probability of being before or after the barrier at a certain time. Moreover, it is shown that the probability propagated across the boundary is $O\left(\delta^{1/2}\right)$ when $\delta \ll \Delta t_1$.

In section 3.1.2, we consider a reflecting barrier removed at some time within an interval $[0, T]$ and reinstated after $t = \delta$, the uncertain time of removal is interpreted as the action of a "demon" on the wall. We obtain the probability density and the total probability for this process (Figures 3.5 & 3.4), where we observe an interpolation between the free particle and the reflecting wall probability densities.

This model allows us to control how many possibilities we want to give to the demon. The variable that module this feature is the number of partitions N; the more we partition the path, the more possibilities the demon has. It is shown that if we increase N, at some point, the probability density begins to saturate (Figure 3.9), i.e., it is not dependent on the number of partitions when this number is large. That is good news if we are interested in taking the limit to the exact path integral $N \to \infty$.

In section 3.2, we address the case of quantum mechanics. Consider a particle in some normalized state ψ_0 initially in the presence of a reflecting wall at $x = 0$. At $t = \Delta t_1$ one wall is removed for a time δ and subsequently reinstated. We found a path integral propagator from where we can compute a wave function for a particle passing through this kind of gate. Other works have studied this case with $\Delta t_1 = 0$, finding applications in measurement theory [22].

Although this work is, in spirit, a solution to a purely theoretical problem, it has the benefit of generality; the broad applicability ranges from a group of ions passing through an ion channel to an electron propagating from a confined domain. More unconventional scenarios can, of course, be proposed.

Appendix A

Gaussian Integral

We aim to solve the following integral

$$I(a) = \int_{-\infty}^{\infty} \mathrm{d}x \; e^{-ax^2}. \tag{A.1}$$

First take the square of I(a)

$$\begin{aligned} I^2 &= \left[\int_{-\infty}^{\infty} \mathrm{d}x \; e^{-ax^2}.\right] \left[\int_{-\infty}^{\infty} \mathrm{d}y \; e^{-ay^2}.\right] \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{d}y \; e^{-\left(x^2+y^2\right)} \end{aligned} \tag{A.2}$$

and use polar coordinates to get

$$I^2 = 2\pi \int_{0}^{\infty} \mathrm{d}r \; re^{-ar^2}. \tag{A.3}$$

Changing variables to $u = r^2$, we obtain

$$I^2 = \pi \int_{0}^{\infty} \mathrm{d}u \; e^{-au} = \pi \left[-\frac{e^{-au}}{a}\right]_{0}^{\infty} = \frac{\pi}{a}, \tag{A.4}$$

which implies that the solution to the gaussian integral is

$$I(a) = \int_{-\infty}^{\infty} \mathrm{d}x \; e^{-ax^2} = \sqrt{\frac{\pi}{a}} \tag{A.5}$$

Appendix B

Computation of the integrals

We have the integrals

$$K_{A1} = \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2 \; K_W(x_0, x_1, \Delta t_1) K_F(x_k, x_2, \delta) K_W(x_2, x_N, \Delta t_2)$$
$$K_{B1} = \int_0^\infty \mathrm{d}x_k \int_0^\infty \mathrm{d}x_2 \; K_W(x_0, x_1, \Delta t_1) K_F(x_k, x_2, \delta) K_W(x_2, x_N, \Delta t_2), \tag{B.1}$$

using eqs. (3.1), (3.2) the problem reduces to solving

$$I_- = \int_0^\infty \mathrm{d}x_1 \int_{-\infty}^0 \mathrm{d}x_2 \; \left(e^{-\frac{(x_0-x_1)^2}{4D\Delta \mathrm{t}_1}} + e^{-\frac{(x_0+x_1)^2}{4D\Delta \mathrm{t}_1}} \right) e^{-\frac{(x_1-x_2)^2}{4D\delta}} \left(e^{-\frac{(x_2-x_N)^2}{4D\Delta \mathrm{t}_2}} + e^{-\frac{(x_2+x_N)^2}{4D\Delta \mathrm{t}_2}} \right)$$
$$I_+ = \int_0^\infty \mathrm{d}x_1 \int_0^\infty \mathrm{d}x_2 \; \left(e^{-\frac{(x_0-x_1)^2}{4D\Delta \mathrm{t}_1}} + e^{-\frac{(x_0+x_1)^2}{4D\Delta \mathrm{t}_1}} \right) e^{-\frac{(x_1-x_2)^2}{4D\delta}} \left(e^{-\frac{(x_2-x_N)^2}{4D\Delta \mathrm{t}_2}} + e^{-\frac{(x_2+x_N)^2}{4D\Delta \mathrm{t}_2}} \right) \tag{B.2}$$

Working out the inner integral and defining

$$c\,(D, \Delta t_1, \delta, \Delta t_2) \equiv \frac{\Delta \mathrm{t}_2}{2\sqrt{D\delta\Delta \mathrm{t}_2(\delta + \Delta \mathrm{t}_2)}}$$
$$d\,(D, x_N, \Delta t_1, \delta, \Delta t_2) \equiv \frac{\delta x_N}{2\sqrt{D\delta\Delta \mathrm{t}_2(\delta + \Delta \mathrm{t}_2)}}$$
$$g\,(x_1, x_N, \Delta t_1, \delta, \Delta t_2) \equiv -\frac{\Delta \mathrm{t}_1 x_N^2 + 2\Delta \mathrm{t}_1 x_1 x_N + 2x_0^2\,(\delta + \Delta \mathrm{t}_2) + x_1^2\,(2\,(\delta + \Delta \mathrm{t}_2) + \Delta \mathrm{t}_1)}{4d\Delta \mathrm{t}_1\,(\delta + \Delta \mathrm{t}_2)}$$

we have

$$I_{\pm} = \int_0^{\infty} \mathrm{d}x_1 \; \frac{\left(e^{\frac{(x_0-x_1)^2}{4D\Delta \mathrm{t}_1}} + e^{\frac{(x_0+x_1)^2}{4D\Delta \mathrm{t}_1}}\right)}{8\pi D\sqrt{\Delta t_1\left(\delta+\Delta \mathrm{t}_2\right)}} \left(1 + e^{\frac{x_1 x_N}{D(\delta+\Delta \mathrm{t}_2)}} \pm \mathrm{erf}\left(cx_1 - d\right) \pm e^{\frac{x_1 x_N}{D(\delta+\Delta \mathrm{t}_2)}} \mathrm{erf}\left(cx_1 + d\right)\right) \exp\left(g\right). \tag{B.3}$$

Defining

$$f_n(a,b,c,d) = \int_0^{\infty} \mathrm{d}x \; x^n e^{-ax^2+bx} \mathrm{erf}\left(cx+d\right) \tag{B.4}$$

we note that eq. (B.3) contains integrals of the form f_0. From the integral tables we get

$$\begin{aligned} f_1(a,b,c,d) = & \frac{e^{\frac{b^2}{4a}}}{4a}\left(\frac{4\sqrt{\pi}b\left(T\left(\frac{2ad+bc}{\sqrt{2}\sqrt{a(a+c^2)}}, \frac{\sqrt{a}(2cd-b)}{2ad+bc}\right) - T\left(\frac{b}{\sqrt{2}\sqrt{a}}, \frac{2\sqrt{a}d}{b}\right)\right)}{\sqrt{a}}\right. \\ & + 2e^{-\frac{b^2}{4a}}\mathrm{erf}(d) + \frac{\sqrt{\pi}b\mathrm{erf}\left(\frac{2ad+bc}{2\sqrt{a(a+c^2)}}\right)}{\sqrt{a}} + \frac{2ce^{-\frac{(-2ad-bc)^2}{4a(a+c^2)}}\,\mathrm{erfc}\left(\frac{2cd-b}{2\sqrt{a+c^2}}\right)}{\sqrt{a+c^2}} \\ & \left. - \frac{2b\left(\tan^{-1}\left(\frac{\sqrt{a}(2cd-b)}{2ad+bc}\right) - \tan^{-1}\left(\frac{2\sqrt{a}d}{b}\right) - \tan^{-1}\left(\frac{c}{\sqrt{a}}\right)\right)}{\sqrt{\pi}\sqrt{a}}\right), \end{aligned} \tag{B.5}$$

where $T(,)$ is the Owen's T function [30]. Integrating by parts using $u = \mathrm{erf}(cx+d)$, $v = e^{-ax^2+bx}$ in the usual prescription, we obtain

$$-2af_1 + bf_0 = -\mathrm{erf}(d) - \frac{2c}{\sqrt{\pi}}\int_0^{\infty} \mathrm{d}x \; e^{-ax^2+bx-(cx+d)}. \tag{B.6}$$

Finally, solving the gaussian integral and inserting (B.5) gives

$$\begin{aligned}
f_0(a,b,c,d) =& \frac{e^{\frac{b^2}{4a}}}{2b}\left(\frac{4\sqrt{\pi}b\left(T\left(\frac{2ad+bc}{\sqrt{2}\sqrt{a}\sqrt{a+c^2}},\frac{\sqrt{a}(2cd-b)}{2ad+bc}\right)-T\left(\frac{b}{\sqrt{2}\sqrt{a}},\frac{2\sqrt{a}d}{b}\right)\right)}{\sqrt{a}}+2e^{-\frac{b^2}{4a}}\mathrm{erf}(d)\right.\\
&+\frac{\sqrt{\pi}b\,\mathrm{erf}\left(\frac{2ad+bc}{2\sqrt{a}\sqrt{a+c^2}}\right)}{\sqrt{a}}+\frac{2ce^{-\frac{(2ad+bc)^2}{4a(a+c^2)}}\mathrm{erfc}\left(\frac{2cd-b}{2\sqrt{a+c^2}}\right)}{\sqrt{a+c^2}}\\
&\left.+\frac{2b\left(-\tan^{-1}\left(\frac{\sqrt{a}(2cd-b)}{2ad+bc}\right)+\tan^{-1}\left(\frac{2\sqrt{a}d}{b}\right)+\tan^{-1}\left(\frac{c}{\sqrt{a}}\right)\right)}{\sqrt{\pi}\sqrt{a}}\right)\\
&-\frac{ce^{\frac{-4ad^2+b^2-4bcd}{4(a+c^2)}}\left(\mathrm{erf}\left(\frac{b-2cd}{2\sqrt{a+c^2}}\right)+1\right)}{b\sqrt{a+c^2}}-\frac{\mathrm{erf}(d)}{b}.
\end{aligned} \tag{B.7}$$

As stated above, $I_\pm$ can be arranged such as it contains only integrals of the form f_0 and ordinary gaussians. Since we already know those results, we can work out $I_\pm$ and therefore, K_{A1} and K_{B_1}. Defining

$$\begin{aligned}
n(D,\Delta\mathrm{t}_1,\Delta\mathrm{t}_2,\delta) &\equiv \frac{1}{8\pi D\sqrt{\Delta\mathrm{t}_1}\sqrt{\delta+\Delta\mathrm{t}_2}}\\
y\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,x_0,\delta,x_N\right) &\equiv -\frac{x_N^2}{4D\left(\delta+\Delta\mathrm{t}_2\right)}-\frac{x_0^2}{4D\Delta\mathrm{t}_1}\\
a\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,\delta\right) &\equiv -\frac{\delta+\Delta\mathrm{t}_1+\Delta\mathrm{t}_2}{4\delta D\Delta\mathrm{t}_1+4D\Delta\mathrm{t}_2\Delta\mathrm{t}_1}\\
b\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,x_0,\delta,x_N\right) &\equiv -\frac{\delta+\Delta\mathrm{t}_1+\Delta\mathrm{t}_2}{4\delta D\Delta\mathrm{t}_1+4D\Delta\mathrm{t}_2\Delta\mathrm{t}_1}\\
c\left(D,\Delta\mathrm{t}_2,\delta,x_N\right) &\equiv \frac{\Delta\mathrm{t}_2}{2\sqrt{\delta D\Delta\mathrm{t}_2\left(\delta+\Delta\mathrm{t}_2\right)}}\\
d\left(D,\Delta\mathrm{t}_2,\delta,x_N\right) &\equiv \frac{\delta x_N}{2\sqrt{\delta D\Delta\mathrm{t}_2\left(\delta+\Delta\mathrm{t}_2\right)}}
\end{aligned}$$

and

$$i_1\left(D,x_0,x_N,\Delta\mathrm{t}_1,\delta,\Delta\mathrm{t}_2\right)\equiv 2n(D,\Delta\mathrm{t}_1,\Delta\mathrm{t}_2,\delta)\sqrt{\frac{\pi D\Delta\mathrm{t}_1\left(\delta+\Delta\mathrm{t}_2\right)}{\delta+\Delta\mathrm{t}_1+\Delta\mathrm{t}_2}}e^{-\frac{(x_N+x_0)^2}{4D(\delta+\Delta\mathrm{t}_1+\Delta\mathrm{t}_2)}}\left(e^{\frac{x_0x_N}{D(\delta+\Delta\mathrm{t}_1+\Delta\mathrm{t}_2)}}+1\right)$$

$$i_2\left(D,x_0,x_N,\Delta\mathrm{t}_1,\delta,\Delta\mathrm{t}_2\right)\equiv n(D,\Delta\mathrm{t}_1,\Delta\mathrm{t}_2,\delta)e^{y(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,x_0,\delta,x_N)}$$

$$\big(f_0\left(-a\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,\delta\right),b\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,-x_0,\delta,-x_N\right),c\left(D,\Delta\mathrm{t}_2,\delta,x_N\right),-d\left(D,\Delta\mathrm{t}_2,\delta,x_N\right)\right)$$

$$+f_0\left(-a\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,\delta\right),b\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,x_0,\delta,-x_N\right),c\left(D,\Delta\mathrm{t}_2,\delta,x_N\right),-d\left(D,\Delta\mathrm{t}_2,\delta,x_N\right)\right)\big)$$

$$i_3\left(D,x_0,x_N,\Delta\mathrm{t}_1,\delta,\Delta\mathrm{t}_2\right)\equiv n(D,\Delta\mathrm{t}_1,\Delta\mathrm{t}_2,\delta)e^{y(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,x_0,\delta,x_N)}$$

$$\big(f_0\left(-a\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,\delta\right),b\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,-x_0,\delta,x_N\right),c\left(D,\Delta\mathrm{t}_2,\delta,x_N\right),d\left(D,\Delta\mathrm{t}_2,\delta,x_N\right)\right)$$

$$+f_0\left(-a\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,\delta\right),b\left(D,\Delta\mathrm{t}_2,\Delta\mathrm{t}_1,x_0,\delta,x_N\right),c\left(D,\Delta\mathrm{t}_2,\delta,x_N\right),d\left(D,\Delta\mathrm{t}_2,\delta,x_N\right)\right)\big)$$

the integrals (B.1), are

$$K_{A1}=i_1-i_2-i_3 \tag{B.8}$$

$$K_{B1}=i_1+i_2+i_3 \tag{B.9}$$

Appendix C

Conservation of the quantum probability

Let $\psi(x,t)$ be a state that satisfies the Schrödinger equation. The time derivative of the probability in the domain $[a,b]$ is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b |\psi(x,t)|^2 \mathrm{d}x &= \frac{\mathrm{d}}{\mathrm{d}t}\int_a^b \psi(x,t)^*\psi(x,t)\mathrm{d}x \\ &= \int_a^b \left(\psi\frac{\partial\psi^*}{\partial t} + \psi^*\frac{\partial\psi}{\partial t}\right).\end{aligned} \tag{C.1}$$

Now consider the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \tag{C.2}$$

and its conjugate

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}, \tag{C.3}$$

if we multiply C.2 by ψ^*, C.3 by ψ and then substract C.2−C.3 we get to

$$\left(\psi\frac{\partial\psi^*}{\partial t} + \psi^*\frac{\partial\psi}{\partial t}\right) = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right), \tag{C.4}$$

inserting this into C.1 and integrating by parts we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b |\psi(x,t)|^2 \mathrm{d}x &= \frac{i\hbar}{2m}\int_a^b \left(\psi^* \frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right) \\ &= \frac{i\hbar}{2m}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right]_a^b = 0. \qquad \text{(C.5)}\end{aligned}$$

The above is satisfied provided

$$|\psi| \to 0 \text{ at the boundaries.} \qquad \text{(C.6)}$$

Bibliography

[1] Robert Brown. *A Brief Account of Microscopical Observations made in the Months of June, July, and August, 1827, on the Particles contained in the Pollen of Plants; and on the General Existence of Active Molecules in Organic and Inorganic Bodies*, volume 1 of *Cambridge Library Collection - Botany and Horticulture*, page 463486. Cambridge University Press, 2015.

[2] A. Einstein. Zur Theorie der *Brownschen* Bewegung. (German) [On the theory of Brownian motion]. 324(2):371–381, 1906.

[3] Paul S. Addison, Bo Qu, Alistair Nisbet, and Gareth Pender. A non-fickian, particle-tracking diffusion model based on fractional brownian motion. *International Journal for Numerical Methods in Fluids*, 25(12):1373–1384, 1997.

[4] G. Hnel. Humidity effects on gravitational settling and brownian diffusion of atmospheric aerosol particles. *Pure and applied geophysics*, page 775797, 1977.

[5] Edmund Bertschinger. Brownian motion of stars, dust, and invisible matter. *AIP Conference Proceedings*, 861(1):97–105, 2006.

[6] David Merritt. Rotational brownian motion of a massive binary. *The Astrophysical Journal*, 568(2):998–1003, apr 2002.

[7] Shawn Means, Alexander J Smith, Jason Shepherd, John Shadid, John Fowler, Richard JH Wojcikiewicz, Tomas Mazel, Gregory D Smith, and Bridget S Wilson. Reaction diffusion modeling of calcium dynamics with realistic er geometry. *Biophysical journal*, 91(2):537–557, 2006.

[8] Upinder S. Bhalla. Signaling in small subcellular volumes. i. stochastic and diffusion effects on individual pathways. *Biophysical Journal*, 87(2):733 – 744, 2004.

[9] Subrahmanyan Chandrasekhar. Stochastic problems in physics and astronomy. *Rev. Mod. Phys.*, 15:1–89, 1943. [,310(1943)].

[10] Jrmie Szeftel. Absorbing boundary conditions for reactiondiffusion equations. *IMA Journal of Applied Mathematics*, 68(2):167–184, 04 2003.

[11] Zeev Schuss. *Theory and Applications of Stochastic Differential Equations*, chapter 4, pages 100–105. John Wiley Sons, 1980.

[12] G. A. Whitmore. First-passage-time models for duration data: Regression structures and competing risks. *Journal of the Royal Statistical Society. Series D (The Statistician)*, 35(2):207–219, 1986.

[13] Sidney Redner. *A guide to first-passage processes*. Cambridge University Press, 2001.

[14] Alun L. Lloyd and Robert M. May. How viruses spread among computers and people. *Science*, 292(5520):1316–1317, 2001.

[15] Marta C. Gonzalez, Cesar Hidalgo, and Albert-Laszlo Barabasi. Understanding individual human mobility patterns. *Nature*, 453:779–82, 07 2008.

[16] Henry C Tuckwell. *Introduction to theoretical neurobiology: volume 2, nonlinear and stochastic theories*, volume 8. Cambridge University Press, 1988.

[17] S. Condamin, O. Bénichou, and M. Moreau. First-passage times for random walks in bounded domains. *Phys. Rev. Lett.*, 95:260601, Dec 2005.

[18] J.M. Harrison. *Brownian Motion and Stochastic Flow Systems*. Robert E. Krieger Publishing Company, 1990.

[19] John FC Kingman. On queues in heavy traffic. *Journal of the Royal Statistical Society: Series B (Methodological)*, 24(2):383–392, 1962.

[20] Donald L. Iglehart and Ward Whitt. Multiple channel queues in heavy traffic. i. *Advances in Applied Probability*, 2(1):150177, 1970.

[21] C.G. Knott. *Life and Scientific Work of Peter Guthrie Tait*. Cambridge University Press, 1911.

[22] A. Marchewka and Z. Schuss. Path-integral approach to the schrödinger current. *Phys. Rev. A*, 61:052107, Apr 2000.

[23] Adam Chaudhry. A general framework for the quantum zeno and anti-zeno effects. *Scientific Reports*, 6, 04 2016.

[24] Gregory F. Lawler and Vlada Limic. *Random Walk: A Modern Introduction*. Cambridge University Press, USA, 2010.

[25] Edward Codling, Michael Plank, and Simon Benhamou. Random walks in biology. *Journal of the Royal Society, Interface / the Royal Society*, 5:813–34, 09 2008.

[26] Motoko Kotani and Toshikazu Sunada. Large deviation and the tangent cone at infinity of a crystal lattice. *Mathematische Zeitschrift*, 254:837–870, 12 2006.

[27] Peter G. Doyle and J. Laurie Snell. *Random Walks and Electric Networks*. Mathematical Association of America, 1984.

[28] Benjamin A. Stickler and Ewald Schachinger. *The Random Walk and Diffusion Theory*, pages 271–295. Springer International Publishing, Cham, 2016.

[29] Jean Philibert. One and a half century of diffusion: Fick, einstein before and beyond. 2006.

[30] Eric W. Weisstein. Owen t-function.