The Hydrodynamic Limit of the Freezing Model

by

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Abstract

In this thesis the hydrodynamic limit of the Freezing Model is studied. The model consists of an integer line on which particles can get frozen to different degrees, analogous to jumping to another integer line, with certain rates and can get unfrozen with certain rates per frozen layer. The main result of the thesis is a proof that the hydrodynamic limit for the Freezing model converges to a system of PDE's describing the particle density for each layer, either the ground layer or a frozen one.
Firstly, it is proven that the position of a random walker in the Freezing Model, appropriately scaled, converges to a so-called Switching Brownian Motion. This together with duality is used in the rest of the proof. Secondly, it is proven that the expectation of the empirical field densities of the layers converges towards the solutions of the aforementioned PDE's. Lastly, it is proven that the variance of the empirical field density converges to 0.
Under an additional diffusive scaling of the system of PDE's for the particle densities, a condition for diffusive behaviour is set up involving the ratio of the freezing and unfreezing rates. It is shown that the PDE's collapse into the heat equation if this condition is satisfied. Finally, the case where the condition is not satisfied is investigated. The model is then no longer memoryless like a Markov process and shows sub-diffusive behaviour. The rescaled position of a single particle then no longer converges to Brownian motion, but to Brownian motion on the time scale on which the particle occupies the ground layer. This time scale is $t^{\beta-1}$ with $1 < \beta < 2$. This grows slower than t for large enough t.
Additionally, simulations in Python were built to show that the model exhibits diffusive or non-diffusive behaviour depending on the jump rates of the process.
Before everything, some mathematical preliminaries about probability theory, Markov theory, random walks and duality are given.

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Introduction

The world around us is made up of an enormous amount of tiny particles moving around and interacting with each other. Each macroscopic physical system, such as a glass of water, contains many. Describing the motion of all the individual particles in such a system is impossible. To solve this problem, the field of statistical mechanics studies macroscopic quantities of large systems of particles by applying statistical methods and probability theory on the microscopic scale, keeping in mind its physical laws that the particles obey. Bernoulli was the one to lay down the basics of statistical physics. In 1738 he published *Hydrodynamica* in which he stated that gases consist of great numbers of molecules moving in every direction, that their collisions on a surface cause pressure and that the experience of heat is simply the kinetic energy of their motion[18].

The area of statistical physics has three founding fathers. Ludwig Boltzmann developed the interpretation of entropy in terms of the number of microstates in a system. James Clerk Maxwell continued on Boltzmanns work and set up probability distributions of such states. For example, he created the first statistical law in physics, describing the proportion of molecules having a velocity in a specific range[2]. In 1902 Gibbs published the book Elementary Principles in Statistical Mechanics[7], in which he formalized statistical mechanics as a general approach to describe all mechanical systems on all scale. These methods still form the foundation of statistical mechanics today.

Most ensembles of particles are analysed in their equilibrium, often an isolated system in a finite volume. A difficult problem in statistical mechanics that remains is analysing complex systems that are not close to their equilibrium state. There is no general theory to describe the behaviour of those systems since they seem to be randomly evolving. A good first step to gain insight into these chaotic arrangements of particles is to consider a simple system of particles that move on a grid following Markovian dynamics, i.e. will move with certain probabilities. The simplest of these models is a particle performing a random walk on a one-dimensional integer line[9]. Even though this is the most basic model, it can still imitate some real life situations, like bacteria either dying off or duplicating themselves, analogous to respectively moving one down or moving one up on the integer line. Often many independent, identically distributed particles are placed in the system and their collective behaviour is inspected.
This basic model of an integer line can be expanded to model more complex systems. For example an exclusion aspect can be added. This means that no two particles can occupy the same site. This model has been introduced in [16] and has been extensively studied, even with extra features such as a two-dimensional environment[19] or a dynamic environment [14]. In this thesis a one-dimensional integer line is used in the model where at each site the particle can get frozen to different degrees and

must 'melt' again before being able to move.

The models of the aforementioned systems are still discrete and on a microscopic scale. We can utilise the models to describe particle behaviour in the continuous real world by scaling the systems towards a macroscopic context. The scaling is in time and space. The parameters that govern the movement of the particles are scaled accordingly to preserve the characteristic movement of the particles. An often used method for this scaling is the hydrodynamic scaling, where space is scaled by N^{-1} and time is scaled by N^2. This is inspired by the fact that a random walker on $\mathbb{Z}$ is on average a distance of $\sqrt{t}$ removed from the starting position at time t, performing Brownian motion[12]. After the scaling, (partial) differential equation(s) are constructed for the movement of small deviations from the macroscopic equilibrium, called local equilibrium. These local equilibriums form a density profile of the particles. The (partial) differential equation(s) that describe the densities profile's evolution through time is called the hydrodynamic limit. This scaling technique is further explained in [5]. For particles performing simple symmetric random walks(i.e. same probability distribution on each site) on a discrete grid, the hydrodynamic limit will result in the heat equation. In this thesis the hydrodynamic scaling is also used as we expect diffusive-like behaviour from the Freezing Model.

Some systems involving Markovian processes, especially those with independent particles, can possess a duality property. This property relates the process to its dual and can greatly simplify some calculations. Especially for symmetric situations the duality links the behaviour of many particles to a single one. By solving the dual problem of a process, information about the original problem can be obtained. This duality approach is widely used in situations involving stochastic processes, for example in the interacting particle systems mentioned earlier or queuing theory.

1.1. Reading Overview

Chapter 2 introduces the mathematical preliminaries of Markov Processes and theory of interacting particles that are necessary for this thesis. In chapter 3 we will prove the hydrodynamic limit of the system and analyse how the parameters of the model will influence the PDE of the macroscopic density profile. In chapter 4 the results of simulations of the Freezing Model will be displayed and discussed. The thesis is concluded by some final remarks.

2

Mathematical Preliminaries

2.1. Introduction

In this chapter we will first provide the mathematical background necessary to understand this thesis. The central subject in this thesis is Markov processes and all the fascinating results you can acquire using the theory surrounding them. Markov processes are sequences of random variables that evolve on probability and measurable spaces. Therefore a lot of real analysis comes into play. Throughout this thesis important facts about real analysis or special spaces will be explained if they are crucial to the proof of some results. Various rigorous and abstract definitions will not be mentioned since they are not vital to deriving the main result of this thesis. These are beyond the scope of this thesis and would only make the central story harder to follow. To keep the thesis clear and concise, it will be assumed that the reader is familiar with the basics of probability theory, i.e. what a random variable is, what a stochastic process is, how conditioning works etc. Even though Markov processes will not be fully covered in depth here, the reader is encouraged to study the field of Markov processes further on their own. For some basic background on Markov theory, the reader is referred to [4]

2.2. Function Spaces

We will first look at the definitions of some spaces of functions that are relevant for this thesis. For a set E, such as $\mathbb{Z}^d$ or $\mathbb{R}^d$,

- $\mathscr{B}(E,\cdot)$ is the space of bounded and measurable functions on E
- $C_0(E,\cdot)$ is the space of continuous functions on E that converge to 0 at $\pm\infty$
- $C_b(E,\cdot)$ is the space of continuous functions on E that are bounded
- $C^n(E,\cdot)$ is the space of continuous functions on E that are n-times differentiable
- $C^\infty(E,\cdot)$ is the space of continuous functions on E that are infinitely differentiable
- $S(\mathbb{R}^n)$ is the Schwartz space or space of functions on $\mathbb{R}^n$ which are rapidly decreasing and whose derivatives are also rapidly decreasing. The formal definition as in [15] is

$$S(\mathbb{R}^n) := \left\{ f \in C^\infty(\mathbb{R}^n |\ \forall \mathbf{a},\mathbf{b} \in \mathbb{N}^n,\ ||f||_{\mathbf{a},\mathbf{b}} < \infty \right\}$$

where $\mathbb{N}^n := \mathbb{N} \times \cdots \times \mathbb{N}$ the n-fold Cartesian product and

$$||f||_{\mathbf{a},\mathbf{b}} := \sup_{\mathbf{x}\in\mathbb{R}^n} \left|\mathbf{x}^{\mathbf{a}}(D^{\mathbf{b}}f)(\mathbf{x})\right|$$

where we use the notation $\mathbf{x}^{\mathbf{a}} := x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n}$ and $D^{\mathbf{b}} := \frac{\partial^{b_1}}{\partial x_1^{b_1}} \frac{\partial^{b_2}}{\partial x_2^{b_2}} \cdots \frac{\partial^{b_n}}{\partial x_n^{b_n}}$

A function in Schwartz can be considered as a function that decays faster to zero for $|x| \to \infty$ than any polynomial of x such that all its derivatives exist everywhere on $\mathbb{R}^n$ and also decay faster to zero than any polynomial of x as $|x| \to \infty$.

- $\mathscr{D}(E,\cdot)$ is the Skorokhod space. It consisits of functions that are right-continuous and have a left limit. The functions are said to be càdlàg. For example all cumulative distribution functions are càdlàg. This space is important in the study of stochastic processes that admit jumps, just like a lot of Markov processes.

where '$\cdot$' is the codomain of the function.. Note that $S(\mathbb{R}^n) \subseteq C_0(E) \subseteq \mathscr{B}(E)$

2.3. Markov Theory

The key characteristic of Markov processes is the fact that they are memory-less, meaning the evolution of the system solely depends on the current state and not on the past states. To mathematically define this property, we first need to introduce the filtration of a probability space:

Definition 2.3.1 *(Filtration) Let $(\Omega,\mathscr{F},P)$ be a probability space and $(T,\mathscr{T})$ be a continuous time space, where $T \subseteq [0,\infty)$. Then a non-decreasing sequence $(\mathscr{F}_t)_{t\in\mathscr{T}}$ of σ-algebras of $\mathscr{F}$*

$$\mathscr{F}_s \subseteq \mathscr{F}_t \subseteq \mathscr{F} \tag{2.1}$$

where $s,t \in T, 0 \le s \le t$, is called a continuous filtration. It can be seen as the events up to time t. If X_t is F_t-measurable for all $t \in T$, then the sequence $\{X_t : t \in T\}$ is said to be adapted to $(\mathscr{F}_t)_{t\in T}$

This is called a discrete filtration if T would have been discrete. In this thesis we only use a continuous time space so the discrete filtration is not relevant.

We can now define the Markov property by using a filtration on time and in doing so capture the memorylessness of a Markov process

Definition 2.3.2 *(Markov property) Let $(\Omega,\mathscr{F},P)$ be a probability space with a continuous filtration $(F_t)_{t\in T}$ and let $(E,\mathscr{E})$ be a measurable space. If for a random process $X_t : \Omega \to E$ with $t \in [0,\infty)$ that is adapted to the filtration it holds that: $\forall S \in \mathscr{E}$, $\forall s,t \in T$ with $0 \le s \le t$,*

$$P(X_t \in S|\mathscr{F}_s) = P(X_t \in S|X_s) \tag{2.2}$$

or equivalently

$$\mathbb{E}\big(f(X_t)|\mathscr{F}_s\big) = \mathbb{E}\big(f(X_t)|X_s\big) \tag{2.3}$$

for $f \in \mathscr{B}(\mathbb{R})$, the space of bounded and measurable functions on $\mathbb{R}$

Remark 2.3.1 *In the context of continuous-time pure jump processes, the memoryless property is coming from the fact that the process jumps at exponentially distributed times.*

Definition 2.3.3 *(Markov Process) Let $(\Omega,\mathscr{F},P)$ be a probability space, $(E,\mathscr{E})$ a measurable space and $(T,\mathscr{T})$ a continuous time space. $\{X_t : t \ge 0\}$ is a Markov process on E if*

- *The paths $t \to X_t$ are right continuous*
- *The process satisfies the Markov property with respect to $\{X_s : 0 \geq s \geq t\}$*

Using the definition of a Markov Process we can define a Markov chain that encaptures how an entire system evolves on which a Markov process takes place

Definition 2.3.4 *(Continuous time Markov Chain) Let (Ω, F, P) be a probability space, $(E, \mathscr{E})$ a discrete space state and $(T, \mathscr{T})$ a continuous time space. Let $\{X_t : t \in T\}$ be a Markov process in the sense of 2.3.3. Then $\{X_t : t \in T\}$ is a continuous time markov chain and is defined by*

- *(i) a probability vector μ on E as an initial distribution*
- *(ii) a rate matrix Q on E which is a function $Q : E^2 \to \mathbb{R}$ such that*
  - $\forall i, j \in E$ *with* $i \neq j, Q_{i,j} \geq 0$
  - $\forall i \in E, \sum_{j \in E, j \neq i} Q_{i,j} = -Q_{i,i}$

The entries of the rate matrix are called *transition rates* and they describe the instantaneous rate at which a continuous-time Markov chain transitions between states.
A lot of Markov processes harbour some symmetry in them. Often positions are indistinguishable and the rate at which you move from one to the other is the same both ways. This is captured in the reversibility definition

Definition 2.3.5 *(Reversible Markov Chain)Take a Markov chain that is continuous in time and let μ be the probability measure on $\boldsymbol{X}$=$\{X_t : t \in T\}$ s.t. μ is invariant on X_0. The Markov chain $\boldsymbol{X}$ is reversible if*

$$\mu_x c_{(x,y)} = \mu_y c_{(y,x)}, \qquad x, y \in S \tag{2.4}$$

In other words, the Markov chain and its reversal in time have the same transition rates. Equation 2.4 is called the detailed balance equation.

2.3.1. Transition probability matrices

Besides the rates with which the Markov chain transitions between states, we can also define a matrix with as entries the probabilities that a chain starting at one site ends up at another on time t.

Definition 2.3.6 *(Transition Probability Matrix) Let $\{X_t : t \in T\}$ be a Continuous Time Markov Chain on E. Then the matrix P_t is called the transition probability matrix at time t and has entries*

$$P_t(x, y) = \mathbb{P}(X_t = y | X_0 = x), \quad x, y \in E \tag{2.5}$$

Remark 2.3.2 *P_0=I, the identity matrix. If P_t does not depend on time, the Markov Chain $X_t : t \geq 0$ is called time homogeneous and the following is true*

$$P_s(x, y) = \mathbb{P}(X_{s+t} = y | X_t = x), \quad x, y \in E, s \in T \tag{2.6}$$

With this matrix we can define the Markov operator, which tells us how a function on the state space changes with the Markov chain

Theorem 2.3.1 *(Markov Operator) Let $\{P_t : t \geq 0\}$ be a set of transition probabilities of the Markov chain $\{X_t : t \geq 0\}$ with state space E and time space T. Suppose $f : E \to \mathbb{R}$ is non-negative or $f \in \mathscr{B}(E)$. Then $\forall t \in T$*

$$P_t f(x) = \sum_{y \in E} P_t(x, y) f(y) = \mathbb{E}(f(X_t) | X_0 = x), \quad x \in E \tag{2.7}$$

defines a Markov operator

Proof: Reader is referred to [4] □

P_t describes the forward evolution of a function along the Markov process $\{X_t : t \geq 0\}$. To this evolution of functions corresponds an evolution of probability measures via the formula $\int f d(\mu P_t) := \int P_t f d\mu$. The measure μP_t is then called the measure at time t when started from the measure μ at $t = 0$.

2.4. Semigroups and Generators

Let $\{P_t : t \geq 0\}$ be a family of Markov operators with an invariant measure μ that satisfy the following conditions:

- (i) For every $t \geq 0$, P_t is a linear operator sending bounded measurable functions on $(E, \mathscr{E})$ to bounded measurable functions
- (ii) $P_0 = Id$, the identity function(*initial condition*)
- (iii) $P_{t+s} = P_t P_s$ for $t, s \geq 0$(*semigroup property*)
- (iv) $P_t(1) = 1$(*mass conservation*)
- (v) If $f \geq 0$, then $P_t f \geq 0$(*positivity preserving*)
- (vi) $\forall f : E \to [0, \infty)$ the function $P_t f$ is continuous

Then $\{P_t : t \geq 0\}$ is called a *Markov semigroup* (see [1]).

We will now introduce another type of semigroup that tells us something about the infinitesimal change of a function. Is is crucial for defining the model of this thesis

Definition 2.4.1 *Let $\{S_t : t \in T\}$ be a continuous semigroup from $C(E) \to C(E)$. The operator*

$$Lf := \lim_{t \to 0^+} \frac{S_t f - f}{t}, \quad f \in D(L) := \left\{ f : \lim_{t \to 0^+} \frac{S_t f - f}{t} \, exists \right\} \tag{2.8}$$

is called the infinitesimal generator of $\{S_t : t \in T\}$

Corollary 2.4.0.1 *For a Markov process $\{X_t : t \in T\}$ with semigroup $\{S_t : t \in T\}$ the generator L is called the Markov generator of $\{X_t : t \in T\}$ and its relation to S_t given by*

$$S_t = e^{tL} \tag{2.9}$$

Proof: see [1] □

Corollary 2.4.0.2 *If $f \in D(L)$, then*

$$\frac{d}{dt} S_t f = S_t L f \tag{2.10}$$

Proof: Let $f \in D(L)$ where L is the infinitesimal generator of $\{S_t : t \in T\}$ in the sense of (2.8). Then

$$\begin{aligned} \frac{d}{dt} S_t f &= \lim_{h \to 0} \frac{S_{t+h} f - S_t f}{h} \\ &= S_t \lim_{h \to 0} \frac{S_h f - f}{h} = S_t L f \end{aligned}$$

where we used the property of a semigroup, i.e. $S_{t+h} = S_t S_h$, in the second equality. □

Remark 2.4.1 *If the state space E is finite, the generator is simply a matrix and e^{tL} is defined as the matrix exponential. In the more general case, when L is a possibly unbounded operator, the exponential is defined via the Hille-Yosida theorem, see [11] for details.*

2.4.1. Random walks and Duality

A lot of systems involve particles that move randomly throughout an environment. The stochastic process of keeping track every step that they make and summing it up is called a random walk. The least complex system for a random walker to move through is a one-dimensional integer line. The walker starts at a certain position and with each step it can move 1 to the right or to the left with certain probabilities. These probabilities do not have to be equal, modelling a bias in direction. This can be used in for example queuing theory, where the rate at which customers arrive is not necessarily the same at which the employee can help them.

The integer line can be expanded into higher dimensions, where in each step the walker can move from their position to neighbouring lattices. This can model particles behaviour in a variety of physical contexts or the process of diffusion.

To analyse the behaviour of the random walker in its environment, we look at the expected value of a test function with the walkers position as its input by simple conditioning

$$\mathbb{E}_x^{\mathrm{RW}}\big(\phi(X_t)\big) = \sum_y P\big(X_t = y | X_0 = x\big)\phi(y) = \sum_y P_t(x,y)\phi(y)$$

where $\{X_t : t \in T\}$ is a Markov process on a state space, $\phi \in S(\mathbb{R})$ is a test function and P_t are the transition probabilities.

These random walks take discrete steps but the position of particles in the real world often take on real values. That is why it is interesting to look at a scaled up version of these discrete walks. For example, the simple symmetric random walk, i.e. equal probabilities to move in every direction, will scale up towards a Brownian motion. This is the motion that particles will exhibit when immersed inside a fluid, for example a big dust particle inside of a gas. The position of the particles will randomly fluctuate due to the collisions with the smaller particles. This process is called a Wiener process and is relevant in numerous contexts within physics, chemistry, etc. and is defined as followed

Definition 2.4.2 *Let $\{X(t) : t \geq 0\}$ be a stochastic process with X_i i.i.d. random variables. The process is called a Wiener process if it satisfies the following conditions:*

- *(i) X_0 a.e.*
- *(ii) X has independent increments, i.e. $\forall\, t \geq 0$, the future increments $X_{t+u} - X_t$, $u \geq 0$ are independent of X_r, $t \geq r \geq 0$*
- *(iii) the increments of X are Gaussian distributed with mean 0 and variance u, i.e. $X_{t+u} - X_t = \mathcal{N}(0,u)$*
- *(iv) X has almost surely continuous paths, i.e. X_t is almost surely continuous in t*

then the process is called a Wiener process.

Proposition 2.4.1 *The generator L of a real-valued Wiener process applied on a function $f \in D(L) = C^2(\mathbb{R})$ is given by*

$$Lf = \frac{1}{2}f'' \tag{2.11}$$

Proof: Note that for a Wiener process $S_t f(x) = \mathbb{E}\big(f(W_t)|W_0 = x\big) = \mathbb{E}\big(f(x + \mathcal{N}(0,t))\big)$, since the increments are normally distributed. Lets Taylor expand this term around x

$$\begin{aligned}\mathbb{E}\big(f(x+\mathcal{N}(0,t))\big) &= \mathbb{E}\left(f(x) + \mathcal{N}(0,t)f'(x) + \frac{1}{2}\mathcal{N}(0,t)^2 f''(x) + O(\mathcal{N}(0,t)^3)\right)\\ &= f(x) + \frac{1}{2}tf''(x) + O(t^{\frac{3}{2}})\end{aligned}$$

Since $\mathbb{E}(\mathcal{N}(0,t)) = 0$ and $\mathbb{E}(\mathcal{N}(0,t)^2) = t$. Then the generator becomes

$$Lf(x) = \lim_{t\to 0^+} \frac{S_t f(x) - f(x)}{t} = \lim_{t\to 0^+} \frac{f(x) + \frac{1}{2}tf''(x) + O(t^{\frac{3}{2}}) - f(x)}{t} = \frac{1}{2}f''(x)$$

□

The systems that are mostly analysed contain a multitude of particles. It is often difficult to keep track of all the particles positions at once and do calculations with them. There is one aspect of random walks that is very useful to resolve this complication. It is called duality. It relates the expected behaviour of a random walk to its dual process. This can be for example the chance that a random walker will reach a certain site related to the inverse walk starting at that site. More relevant for this thesis, duality can be used to describe a system with numerous(possibly infinitely many) independent walkers. It describes expectations of numbers of particles at time $t > 0$ in term of a finite number of particles. More precisely, the expectation of a specific polynomial of degree n in the number of particles can be described in terms of n particles. In this thesis we will use the $n = 1$ case to describe the expected number of particles in terms of a single walker. We will also use the $n = 2$ case to prove that the variance of the density of the system converges to 0.
The duality between two Markov processes is understood in terms of a duality function D and gives a one-to-one relation between the problem and its dual. The duality property is defined as followed

Definition 2.4.3 *(Duality property)Let $S, \tilde{S}$ be the state spaces of the Markov processes $(\eta_t)_{t\geq 0}$ and $(\xi_t)_{t\geq 0}$ respectively. The Markov processes are dual with respect to the duality function $D : Sx\tilde{S} \to \mathbb{R}$ if $\forall\, t \geq 0, \forall \eta \in S, \forall \xi \in \tilde{S}$*

$$\mathbb{E}_\eta(D(\xi, \eta_t)) = \mathbb{E}_\xi(D(\xi_t, \eta)) \tag{2.12}$$

holds. If $S = \tilde{S}$, then the Markov process is called self-dual.

3

The Freezing Model

3.1. Introduction

The Freezing Model investigates what the behaviour of particles is in a complicated environment, where they can get frozen for an amount of time before unfreezing and moving again. The model consists of particles that perform random walks and an infinite 'bunkbed' in which the particles can 'sleep'.

The main concept of the Freezing Model is that these particles can get frozen to different degrees. After getting frozen, they have to wait an exponential amount of time before they 'melt' and are able to move again. The higher the degree of freezing, the longer they are frozen on average.

The aim of studying this model is to gain insight into the movement of random walkers in special environments. The Freezing Model can imitate phenomena like a special kind of diffusion or bacteria reproduction and genetic variability in unfavourable environments(see [13]). The model can be a first step in investigating what happens when particles can get 'trapped' at certain cites. This can be expanded by an inhomogeneous trapping environment, where the trapping depth is different per site. Such a system, for example the Bouchaud trap model[3], will exhibit sub-diffusive behaviour. The Freezing Model can be expanded to this sort of system by letting the average degree that the particles get frozen by vary between sites.
These kinds of systems are very complex and even though the Freezing Model is relatively simple, it can act as a first step towards understanding the behaviour of these systems.

3.2. Definition of the Freezing Model

Consider a continuous time Markov Process which operates on a probability space (Ω, $\mathscr{F}$, P). This process, denoted by $\mathbf{X}$:=$\{(X_t, i_t) : t \in T = [0,\infty)\}$, has a countable infinite set of copies of the one-dimensional integer line as the state space, S=$\mathbb{Z} \times \mathbb{N}_0$ and has a continuous time space T.

At time t=0 a finite amount of particles are placed on the lattice. These particles are performing identical independent random walks with the following jump rates:

- a particle at layer 0 jumps from x to x$\pm$1 at rate 1
- a particle at x jumps from layer 0 to layer i at rate γ_i^u
- a particle at x jumps from layer i to layer 0 at rate γ_i^d

Written down formally, the jump rates from (x,i) to (y,j) of the random walk are:

$$c_{((x,i),(y,j))} = \begin{cases} 1, & \text{if i=j=0 and y=x}\pm 1 \\ \gamma_j^u, & \text{if i=0, j}\neq 0 \text{ and y=x} \\ \gamma_i^d, & \text{if i}\neq 0, \text{ j=0 and y=x} \\ 0, & \text{otherwise} \end{cases} \tag{3.1}$$

The jump rates determine the distribution of the waiting time on each site. The mean waiting time is equal to the sum of the jump rates away from that site, i.e.

$$\tau_{\text{jump}} \sim \exp(c_{(x,i)}), \quad \text{where } c_{(x,i)} = \sum_{(y,j)\neq(x,i)} c_{((x,i),(y,j))}$$

For the Freezing Model this becomes

$$\tau_{\text{jump}} \sim \exp(c_{(x,i)}), \quad \text{where } c_{(x,i)} = \begin{cases} 2 + \sum_{n=1}^{\infty} \gamma_n^u & \text{, if i=0} \\ \gamma_i^d & \text{, otherwise} \end{cases} \tag{3.2}$$

Using the jump rates, we can calculate the generator of the process

$$\begin{aligned} Gf(x,i) &= \sum_{(y,j)\in\mathbb{Z}\times\mathbb{N}_0} c_{((x,i),(y,j))}(f(y,j)-f(x,i)) \\ &= \begin{cases} f(x+1,0) - 2f(x,0) + f(x-1,0) + \sum_{i\in\mathbb{N}} \gamma_i^u (f(x,i)-f(x,0)), \text{ if i=0} \\ \gamma_i^d (f(x,0)-f(x,i)), \text{ otherwise} \end{cases} \end{aligned} \tag{3.3}$$

We then consider the particles moving independently according to the generator (3.3). Initially at each (x,i) we place $\eta(x,i)$ particles and then call the number of particles at time t $\eta_t(x,i)$ and η_t the whole configuration of these particle numbers. η_t is a Markov process and defined as followed

$$\eta_t = (\eta_t(x,i))_{(x,i)} \in \mathscr{X} \tag{3.4}$$

which has a state space $\mathscr{X} = \mathbb{N}^{\mathbb{Z}\times\mathbb{N}}$ and its generator is given by:

$$\mathscr{L} = \mathscr{L}^{move} + \mathscr{L}^{swtich} \tag{3.5}$$

where

$$\mathscr{L}^{move} f(\eta) = \sum_{x\in\mathbb{Z}} \begin{pmatrix} \eta(x,0)\left(f(\eta - \delta_{(x,0)} + \delta_{(x+1,0)}) - f(\eta)\right) \\ +\eta(x,0)\left(f(\eta - \delta_{(x,0)} + \delta_{(x-1,0)}) - f(\eta)\right) \end{pmatrix} \tag{3.6}$$

and

$$\mathscr{L}^{switch} f(\eta) = \sum_{x\in\mathbb{Z}} \sum_{i\in\mathbb{N}} \begin{pmatrix} \gamma_i^d \eta(x,i)\left(f(\eta - \delta_{(x,i)} + \delta_{(x,0)}) - f(\eta)\right) \\ +\gamma_i^u \eta(x,0)\left(f(\eta - \delta_{(x,0)} + \delta_{(x,i)}) - f(\eta)\right) \end{pmatrix} \tag{3.7}$$

for local functions $f : \mathbb{Z}\times\mathbb{N}_0 \to \mathbb{R}$

We will now introduce some notation that is used later on:

- $\mathbb{E}_\eta$ denotes the expectation starting from a fixed initial configuration of particles η
- $\mathbb{E}_\mu = \int \mathbb{E}_\eta d\mu(\eta)$ denotes the expectation starting from an initial configuration η which is itself distributed according to μ

3.3. Hydrodynamic Limit

The behaviour of individual particles is now defined. Each particle is moving around independently. Therefore it is relatively easy to study the collective behaviour of all particles and see how the model scales up to a continuous space instead of a discrete one. This invites us to study the hydrodynamic limit of the system, which shows us the macroscopic behaviour of the system. We will first make some assumptions about the probability measures we use in the model at t=0

Assumption 3.3.1 ***[Compatible initial conditions]****Let $\tilde{\rho}_i \in C_b(\mathbb{R};\mathbb{R}_+)$ for $i \in \mathbb{N}_0$ be the initial density profiles of the layers. The sequence of probability measures $(\mu_N)_{N\in\mathbb{N}}$ on $\mathscr{X}$ is compatible with the initial conditions if:*

- *(i) For all $i \in \mathbb{N}, \phi \in C_c^\infty(\mathbb{R})$ and $\delta > 0$,*

$$\lim_{N\to\infty} \mu_N\left(\left|\langle X_0^{i,N}, \phi\rangle - \int_{\mathbb{R}} \tilde{\rho}_i(x)\phi(x)dx\right| > \delta\right) = 0 \tag{3.8}$$

- *(ii) There exist a constant $C < \infty$ such that*

$$\sup_{(x,i)\in\mathbb{Z}\times\mathbb{N}} \mathbb{E}_{\mu_N}\left(\frac{\eta(x,i)^2}{\alpha_i^2}\right) \leq C \tag{3.9}$$

Note that $\langle X_0^{i,N}, \phi\rangle = \frac{1}{N}\sum_{x\in\mathbb{Z}} \eta_0(x,i)\phi(\frac{x}{N})$.

With these compatible conditions we can now define the hydrodynamic limit for the Freezing Model. First the result of the hydrodynamic limit is given, then the definition and meaning of this limit are further explained and finally the limit will be proven. In this chapter we will obtain the following result:

Theorem 3.3.1 *Let $\tilde{\rho}_i \in C_b(\mathbb{R};\mathbb{R}_+)$ for $i \in \mathbb{N}_0$ be the initial density profiles of the layers and $(\mu_N)_{N\in\mathbb{N}}$ be a sequence of compatible initial conditions such that $\int \eta(y)d\mu_N = \rho(\frac{y}{N})$. Let $\mathbb{P}_{\mu_N}$ be the law of the measure valued-process:*

$$\{X_t^N : t \geq 0\}, \qquad X_t^N := (X_t^{i,N})_{i\in\mathbb{N}_0}$$

where

$$X_t^{i,N} := \frac{1}{N}\sum_{x\in\mathbb{Z}} \eta_{tN^2}(x,i)\delta\left(\frac{x}{N}\right)$$

is the empirical field density for a single layer. Given that the expectation of a rescaled Markov process of a random walker in the Freezing Model converges to the expectation of Switching Brownian Motion as in equation (3.15), in other words

$$\mathbb{E}^{RW}_{(\frac{x}{N},i)}\left(f\left(\frac{X_{tN^2}}{N}, i\right)\right) \to \mathbb{E}^{SBM}_{(\frac{x}{N},i)}\left(f(B_t, i_t)\right)$$

As a consequence for $\phi \in S(\mathbb{R})$ a test function, the following holds $\forall\, T, \delta > 0$

$$\lim_{N\to\infty} \mathbb{P}_{\mu_N}\left(\sup_{t\in[0,T]}\left|\langle X_t^{i,N}, \phi\rangle - \int_{\mathbb{R}} \rho_t(x,i)\phi(x)dx\right| > \delta\right) = 0, i \in \mathbb{N}_0 \tag{3.10}$$

or equivalently

$$\mathbb{E}_{\mu_N}\left(\mathbb{E}_\eta\left(\frac{1}{N}\sum_{x\in\mathbb{Z}} \eta_{tN^2}(x,i)\phi\left(\frac{x}{N}\right)\right)\right) \underset{N\to\infty}{\to} \int_{\mathbb{R}} \rho_t(x,i)\phi(x)dx$$

and

$$Var_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi\left(\frac{x}{N}\right)\right)\underset{N\to\infty}{\to}0$$

where $\rho_t(x,i)$ are the unique continuous and bounded solutions of the system:

$$\begin{cases}\frac{\partial\rho_t(x,0)}{\partial t}=\Delta\rho_t(x,0)+\sum_{i\geq1}\left(\gamma_i^d\rho_t(x,i)-\gamma_i^u\rho_t(x,0)\right)\\ \frac{\partial\rho_t(x,i)}{\partial t}=\gamma_i^u\rho_t(x,0)-\gamma_i^d\rho_t(x,i)\end{cases}\tag{3.11}$$

with initial conditions

$$\rho_0(x,i)=\tilde{\rho}(x,i),i\in\mathbb{N}_0\tag{3.12}$$

3.3.1. Meaning of the Hydrodynamic Limit

The concept of the hydrodynamic limit is to describe(i.e. define and prove) the macroscopic behaviour of the densities of particles after an appropriate rescaling of time and space. In this process it turns the discrete space system into a continuous space system.
Recall that a finite amount of particles are placed in the system at the start. Lets say without loss of generality that $H<\infty$ is that amount. Every particle will perform an independent random walk through the lattice, i.e. $\{X_t:t\geq0\}$. Then configuration can be written down as $\{\eta_t:t\geq0\}=\{X_t^i:t\geq0,i\in\{1,2,...,H\}\}$, where $\eta_t(x,i)=\sum_{k=1}^{H}I(X_t^k=(x,i))$ denotes the number of particles at site (x,i) and time t. $\eta_t(x,i)$ has the Markov property given that the random walkers do.

The first step to the hydrodynamic limit is to define a sequence of discrete spaces $U_N\subseteq\mathbb{Z},N\in\mathbb{N}$ with $|U_N|=N$ such that for every $x\in\mathbb{R}$ there exist a sequence $\{\frac{x_N}{N}:x_N\in U_N,N\in\mathbb{N}\}$ with $\frac{x_N}{N}\to x$ as $N\to\infty$. This is possible due to the fact that the rationals are dense in $\mathbb{R}$[10]. The second step is observing the macroscopic point x instead of the integer microscopic points x_N using a sequence of empirical field densities for a single layer

$$X_t^{i,N}:=\frac{1}{|U_N|}\sum_{x\in\mathbb{Z}}\eta_{t\theta_N}(x,i)\delta\left(\frac{x}{N}\right)$$

where$\delta(x)$ is the Kronecker delta function and θ_N is the time scaling factor. Since we expect diffusion in our model, we choose $\theta_N=N^2$. A detailed explanation for this factor can be found in section A.1. We will investigate how this empirical field density will act on a test function, $\phi\in S(\mathbb{R})$, the Schwartz space on $\mathbb{R}$. Thus the object that will be looking at for the hydrodynamic limit is,

$$\langle X_t^{i,N},\phi\rangle=\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}\phi\left(\frac{x}{N}\right)$$

using the fact that $\langle\delta\left(\frac{x}{N}\right),\phi\rangle=\phi\left(\frac{x}{N}\right)$.
We will now introduce the macroscopic density function, which is a measurable function $\rho_t(x,i):\mathbb{R}\times\mathbb{N}\to\mathbb{R}_{\geq0}$. A sequence of probability measures (μ_N) is assigned to this density profile at t=0 so that they will be compatible in the sense of equation (3.8. The hydrodynamic limit are the PDE's of these $\rho_t(x,i)$ when they satisfy equation (3.10). These PDE's will therefor describe the behaviour of the whole system.

3.3.2. Proof of the Hydrodynamic Limit

Before we prove equation (3.10), we will first introduce a duality relation between the configuration process and a single random walker. Due to this relation we can analyse the behaviour of the configuration by analysing the expected behaviour of a single random walker within the configuration. This technique greatly simplifies some calculations we need to do. To prove the duality property we need the detailed balance equation of our model in a slightly different form:

Remark 3.3.1 *The detailed balance equation (2.4) in the case of the Freezing model becomes:*

$$\mu(0)\gamma_i^u = \mu(i)\gamma_i^d$$

or:

$$\frac{\mu(i)}{\mu(0)} = \frac{\gamma_i^u}{\gamma_i^d} := \alpha_i$$

Another form of the detailed balance equation is:

$$\mu(i)P_t((x,i),(y,j)) = \mu(j)P_t((y,j),(x,i))$$

Dividing both sides by $\mu(0) \neq 0$ *we get:*

$$\alpha_i P_t((x,i),(y,j)) = \alpha_j P_t((y,j),(x,i)) \tag{3.13}$$

Now we can prove the duality property of the Freezing Model

Proposition 3.3.1 *(Duality property For each* $\eta \in \mathscr{X}$ *and* $(x,i) \in S$

$$\mathbb{E}_\eta\left(\frac{\eta_t(x,i)}{\alpha_i}\right) = \mathbb{E}^{RW}_{(x,i)}\left(\frac{\eta_t(X_t,i_t)}{\alpha_{i_t}}\right) \tag{3.14}$$

where $\alpha_i = \frac{\gamma_i^u}{\gamma_i^d}$.

Proof: Starting from the left-hand side:

$$\begin{aligned}
\mathbb{E}_\eta\left(\frac{\eta_t(x,i)}{\alpha_i}\right) &= \mathbb{E}\left(\sum_{(y,j)\in S}\sum_{k=1}^{\eta(y,j)} I(X_t^{k,(y,j)}(t) = (x,i))\frac{1}{\alpha_i}\right) \\
&= \sum_{(y,j)\in S}\sum_{k=1}^{\eta(y,j)} P_t((y,j),(x,i))\frac{1}{\alpha_i} \\
&\overset{(3.13)}{=} \sum_{(y,j)\in S}\sum_{k=1}^{\eta(y,j)} P_t((x,i),(y,j))\frac{1}{\alpha_j} \\
&= \sum_{(y,j)\in S}\eta(y,j)P_t((x,i),(y,j))\frac{1}{\alpha_j} = \mathbb{E}^{\mathrm{RW}}_{(x,i)}\left(\frac{\eta_t(X_t,i_t)}{\alpha_{i_t}}\right)
\end{aligned}$$

where we used the linearity of the expectation value and the fact that the expectation value of the indicator function of a random walk is the transition probability from starting site to the site that the indicator is located on, i.e. $\mathbb{E}[I(X^{(y,j)}(t) = (x,i))] = P_t((y,j),(x,i))$, in the first step. In the second step we used the detailed balance equation. □

With this duality property now proven, we can now prove that the expectation of the empirical field density converges to an integrand with $\rho_t(i)$ that satisfies equations (3.11). After that we will prove that the variance of the empirical field density will converge to 0. These two facts together prove equation (3.10). To prove the convergence of the expectation, we will first prove that the expectation of a random walker in the Freezing Model will converge towards the expectation of a Switching Brownian Motion.

Convergence of the process generator

For any $N \geq 0$ the rescaled dual R.W. generator is given by

$$G_N f(x,i) = \begin{cases} N^2\left(f(x+1,0) - 2f(x,0) + f(x-1,0) + \sum_{n\in\mathbb{N}} \frac{\gamma_n^u}{N^2}(f(x,n) - f(x,0))\right), \text{ if i=0} \\ N^2 \frac{\gamma_i^d}{N^2}(f(x,0) - f(x,i)), \text{ otherwise} \end{cases}$$
$$= \begin{cases} N^2\left(f(x+1,0) - 2f(x,0) + f(x-1,0)\right) + \sum_{n\in\mathbb{N}} \gamma_n^u (f(x,n) - f(x,0)), \text{ if i=0} \\ \gamma_i^d (f(x,0) - f(x,i)), \text{ otherwise} \end{cases}$$

We will show that the random walker with this generator will converge to a switching Brownian motion(SBM) $(B_t, i_t) \in \mathbb{R} \times \mathbb{N}$ with a generator given by

$$\mathscr{L}_{SBM} f(x,i) = \begin{cases} \Delta f(x,0) + \sum_{n\in\mathbb{N}} \gamma_n^u (f(x,n) - f(x,0)), \text{ if i=0} \\ \gamma_i^d (f(x,0) - f(x,i)), \text{ otherwise} \end{cases} \tag{3.15}$$

Proposition 3.3.2 *For each $T \geq 0$ and $f \in C_c^2(\mathbb{R})$*

$$\lim_{N\to\infty} \sup_{t\in[0,T]} \sup_{(x,i)\in\mathbb{Z}\times\mathbb{N}_0} \left| \mathbb{E}^{RW}_{(\frac{x}{N},i)} \left[f\left(\frac{X_{tN^2}}{N}, i\right)\right] - \mathbb{E}^{SBM}_{(\frac{x}{N},i)}[f(B_t, i_t)] \right| = 0 \tag{3.16}$$

Proof: Let $f(\cdot,i) \in C_c^2(\mathbb{R})$ s.t. $\sup_{(x,i)\in\mathbb{Z}\times\mathbb{N}} |f(x,i)| < \infty$. Define

$$f_N : \frac{\mathbb{Z}}{\mathbb{N}} \times \mathbb{N}_0 \to \mathbb{R}$$
$$f_N(\frac{x}{N}, i) := f(\frac{x}{N}, i)$$

Then

$$\lim_{N\to\infty} \sup_{(x,i)\in\mathbb{Z}\times\mathbb{N}_0} \left| f_N(\frac{x}{N}, i) - f(\frac{x}{N}, i) \right| = 0$$

and since $\lim_{N\to\infty} N^2(f(x+\frac{1}{N},i) - 2f(x,i) + f(x-\frac{1}{N},i)) \to \Delta f(x,i)$,

$$\lim_{N\to\infty} \sup_{(x,i)\in\mathbb{Z}\times\mathbb{N}_0} \left| G_N f_N(\frac{x}{N}, i) - \mathscr{L}_{SBM} f(\frac{x}{N}, i) \right| = 0$$

The results follows from the fact that the expectation of the processes will converge to the same value if the generators converge. □

Step 1: Convergence of the expectation

$$\mathbb{E}_{\mu_N}\left(\mathbb{E}_\eta\left(\frac{1}{N}\sum_{x\in\mathbb{Z}} \eta_{tN^2}(x,i)\phi\left(\frac{x}{N}\right)\right)\right)$$
$$= \mathbb{E}_{\mu_N}\left(\mathbb{E}_\eta\left(\frac{1}{N}\sum_{x\in\mathbb{Z}} \frac{\eta_{tN^2}(x,i)}{\alpha_i}\phi\left(\frac{x}{N}\right)\alpha_i\right)\right)$$
$$= \mathbb{E}_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}} \mathbb{E}_\eta\left(\frac{\eta_{tN^2}(x,i)}{\alpha_i}\right)\phi\left(\frac{x}{N}\right)\alpha_i\right)$$
$$= \mathbb{E}_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}} \mathbb{E}^{\mathrm{RW}}_{(x,i)}\left(\frac{\eta(X_{tN^2}, i_{tN^2})}{\alpha_{i_{tN^2}}}\right)\phi\left(\frac{x}{N}\right)\alpha_i\right)$$

using duality in the last step. Using the fact that $\mathbb{E}_{\mu_N}[\eta(x,i)] = \rho(\frac{x}{N}, i)$, we get the following

$$= \frac{1}{N}\sum_{x\in\mathbb{Z}} \alpha_i \mathbb{E}^{\mathrm{RW}}_{(x,i)}\left(\frac{\rho(\frac{X_{tN^2}}{N}, i_{tN^2})}{\alpha_{i_{tN^2}}}\right)\phi\left(\frac{x}{N}\right)$$
$$\underset{N\to\infty}{\to} \int_{\mathbb{R}} \alpha_i \mathbb{E}^{\mathrm{SBM}}_{(x,i)}\left(\frac{\rho(B_t, i_t)}{\alpha_{i_t}}\right)\phi(x)\,dx$$

Using equation (3.16).
We then have that

$$\rho_t(x,i) := \alpha_i \mathbb{E}^{\mathrm{FM}}_{(x,i)}\left(\frac{\rho(B_t, i_t)}{\alpha_{i_t}}\right)$$

satisfies equations (3.11). The derivation for these PDE's is in section A.2.

Step 2: Control of the variance and convergence in $\mathscr{L}^2$ of the density field

We will first prove duality for two particles since we will use this to proof that the variance converges to zero.

Theorem 3.3.2 ***(Duality for two particles)*** *Let $\{X_t : t \geq 0\}$ and $\{Y_t : t \geq 0\}$ be two random walkers in the Freezing Model. Then the following dual duality holds:*

$$\mathbb{E}_\eta\left(\frac{\eta_t(x,i)}{\alpha_i}\frac{\eta_t(y,j)}{\alpha_j}\right) = \mathbb{E}^{RW's}_{((x,i),(y,j))}\left(\frac{\eta(X_t,i_t)}{\alpha_{i_t}}\frac{\eta(Y_t,j_t)}{\alpha_{j_t}}\right) - \sum_{(x',i')}\frac{\eta(x',i')}{\alpha^2_{i'}}P_t((x,i),(x',i'))P_t((y,i),(x',i')) \tag{3.17}$$

Proof: The proof follows similar steps to the proof of the single particle duality and uses the fact that the random walkers are independent of each other. The full proof is in the Appendix, see section (A.4). □

Secondly we will need some facts about Schwartz functions

Theorem 3.3.3 *Let $f, g \in S(\mathbb{R})$ and let H be a bounded smooth function with bounded smooth derivatives. Then the following two statements hold*

- *(i) $f + g \in S(\mathbb{R})$*
- *(ii) $fH \in S(\mathbb{R})$*

Proof: Lets prove statement (i) first. Let $f, g \in S(\mathbb{R})$. Then $\forall a, b \in \mathbb{N}$

$$||f||_{a,b} = \sup_{x\in\mathbb{R}} |x^a (D^b f)(x)| < \infty$$

and

$$||g||_{a,b} = \sup_{x\in\mathbb{R}} |x^a (D^b g)(x)| < \infty$$

where $D^b f$ is the derivative operator acting on f b times. Then the following holds

$$||f+g||_{a,b} = \sup_{x\in\mathbb{R}} |x^a (D^b (f+g))(x)| \leq \sup_{x\in\mathbb{R}} |x^a (D^b f)(x)| + \sup_{x\in\mathbb{R}} |x^a (D^b g)(x)| < \infty$$

where we used linearity of the derivative operator and the triangle inequality. This means that $||f + g||_{a,b} < \infty$ and thus $f + g \in S(\mathbb{R})$. For the proof of statement (ii) the reader is referred to [15].

Now we can start with the proof for the variance of the empirical field density of our model. We will first make an assumption about the configurations:

Assumption 3.3.2

$$\int \eta(x,i)\eta(y,j)d\mu_N = \begin{cases} \rho(\frac{x}{N},i))\rho(\frac{y}{N},j), \text{if } (x,i) \neq (y,j) \\ \rho_2(\frac{x}{N},i), \text{if } (x,i)=(y,j) \end{cases}$$

where $\rho^2(\frac{x}{N},i) \leq \rho_2(\frac{x}{N},i) \leq C\alpha_i^2 < \infty$ using equation (3.9).

$$\mathrm{Var}_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N})\right) = \mathbb{E}_{\mu_N}\left(\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N}\right)^2\right) - \mathbb{E}_{\mu_N}\left(\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N}\right)\right)^2$$

We will calculate the second term first:

$$\begin{aligned}\mathbb{E}_{\mu_N}\left(\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N})\right)\right) &= \frac{1}{N}\sum_{x\in\mathbb{Z}}\phi(\frac{x}{N})\mathbb{E}_{\mu_N}\left(\eta_{tN^2}(x,i)\right) \\ &= \frac{1}{N}\sum_{x\in\mathbb{Z}}\phi(\frac{x}{N}\int\sum_{(x',i')}\eta(x',i')P_{tN^2}((x,i),(x',i'))\frac{\alpha_i}{\alpha_{i'}}d\mu_N \\ &= \frac{1}{N}\sum_{x\in\mathbb{Z}}\phi(\frac{x}{N})\sum_{(x',i')}\rho(\frac{x'}{N},i')P_{tN^2}((x,i),(x',i'))\frac{\alpha_i}{\alpha_{i'}}\end{aligned}$$

where we used the duality property in the second equality and $\mathbb{E}_{\mu_N}[\eta(x,i)] = \rho(\frac{x}{N},i)$ in the last step. so

$$\begin{aligned}\left(\mathbb{E}_{\mu_N}\left(\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N})\right)\right)\right)^2 &= \left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\phi(\frac{x}{N})\sum_{(x',i')}\rho(\frac{x'}{N},i')P_{tN^2}((x,i),(x',i'))\frac{\alpha_i}{\alpha_{i'}}\right)^2 \\ &= \frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\sum_{(x',i')}\sum_{(y',j')}P_t((x,i),(x',i'))P_t((y,i),(y',j'))\rho(\frac{x'}{N},i')\rho(\frac{y'}{N},j') + O(1)\end{aligned}$$

where the O(1) term is related to the fact taht we will discard the x=y terms as $N \to \infty$. We may do this because the third and fourth sum are finite since $P_t(\cdot) \leq 1$ and the densities are bounded by assumptions. This together with the fact that $\frac{1}{N}\sum_x \phi(\frac{x}{N})^2 \to \int_{\mathbb{R}}\phi(x)^2dx < \infty$ and the extra $\frac{1}{N}$ factor will make the x=y terms vanish in the limit when N goes to infinity.
Now we will calculate the first term of the variance:

$$\begin{aligned}&\mathbb{E}_{\mu_N}\left(\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N}\right)^2\right) \\ &= \frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\alpha_i^2\mathbb{E}_{\mu_N}\left(\frac{\eta_{tN^2}(x,i)}{\alpha_i}\frac{\eta_{tN^2}(y,i)}{\alpha_i}\right) + O(1)\end{aligned}$$

where the O(1) again comes from the x=y terms that we can discard again as $N \to \infty$. We may do this because

$$\frac{1}{N^2}\sum_x \phi(\frac{x}{N})^2\alpha_i^2\mathbb{E}_{\mu_N}\left(\frac{\eta_{tN^2}(x,i)^2}{\alpha_i^2}\right) \leq \frac{1}{N^2}\sum_x \phi(\frac{x}{n})^2\alpha_i^2 C \underset{N\to\infty}{\to} 0$$

where we used (3.9) and the fact that $\frac{1}{N}\sum_x C\alpha_i^2\phi(\frac{x}{N})^2 \underset{N\to\infty}{\to} \int_{\mathbb{R}} C\alpha_i^2\phi(x)^2 < \infty$, $C < \infty$ and $\alpha_i < \infty$.

Now using equation (3.17) the top equation is

$$= \frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\frac{\alpha_i^2}{\alpha_{i'}\alpha_{j'}}\sum_{(x',i')}\sum_{(y',j')}P_t((x,i),(x',i'))P_t((y,i),(y',j'))\int\eta(x',i')\eta(y',j')d\mu_N$$
$$-\frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\frac{\alpha_i^2}{\alpha_{i'}^2}\sum_{(x',i')}P_t((x,i),(x',i'))P_t((y,i),(x',i'))\int\eta(x',i')d\mu_N$$

$$= \frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\sum_{(x',i')\neq(y',j')}\frac{\alpha_i^2}{\alpha_{i'}\alpha_{j'}}P_t((x,i),(x',i'))P_t((y,i),(y',j'))\rho(\frac{x'}{N},i')\rho(\frac{y'}{N},j')$$
$$+\frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\sum_{(x',i')}\frac{\alpha_i^2}{\alpha_{i'}^2}P_t((x,i),(x',i'))P_t((y,i),(x',i'))\rho_2(\frac{x'}{N},i')$$
$$-\frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\sum_{(x',i')}\frac{\alpha_i^2}{\alpha_{i'}^2}P_t((x,i),(x',i'))P_t((y,i),(x',i'))\rho(\frac{x'}{N},i')$$

Where we used the assumptions about the configurations on both integrals. The total variance then becomes

$$\mathrm{Var}_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N})\right)$$
$$= \frac{1}{N^2}\sum_{x\neq y}\phi(\frac{x}{N})\phi(\frac{y}{N})\sum_{(x',i')}\frac{\alpha_i^2}{\alpha_{i'}^2}P_t((x,i),(x',i'))P_t((y,i),(x',i'))\left(\rho_2(\frac{x'}{N},i')-\rho^2(\frac{x'}{N},i')-\rho(\frac{x'}{N},i')\right)$$

Define $\xi_t(\frac{x'}{N},i') := \sum_x\left|\phi(\frac{x}{N})\right|P_t((x,i),(x',i')$. then the following holds

$$\mathrm{Var}_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N})\right)\leq\frac{1}{N^2}\sum_{(x',i')}\frac{\alpha_i^2}{\alpha_{i'}^2}\left(\rho_2(\frac{x'}{N},i')-\rho^2(\frac{x'}{N},i')-\rho(\frac{x'}{N},i')\right)\xi_t(\frac{x'}{N},i)^2$$

We know

$$\frac{1}{N}\sum_{(x',i')}\frac{\alpha_i^2}{\alpha_{i'}^2}\left(\rho_2(\frac{x'}{N},i')-\rho^2(\frac{x'}{N},i')-\rho(\frac{x'}{N},i')\right)\xi_t(\frac{x'}{N},i)^2\to\int_{\mathbb{R}}\frac{\alpha_i^2}{\alpha_{i'}^2}\left(\rho_2(x',i')-\rho^2(x',i')-\rho(x',i')\right)\xi_t(x',i)^2dx'$$

ξ is a convolution of $|\phi|\in S(\mathbb{R})$ and the transition probabilities P_t. The transition probabilities are all smaller or equal to 1 and will not make jumps in time since the system will change smoothly through time. This means that the P_t's are smooth and bounded and so are their derivatives. Using Theorem 3.3.3 we can say that ξ a function in the Schwartz-Space on $\mathbb{R}$. Since the configuration is bounded and smooth everywhere, the densities are also bounded and smooth together with all their derivatives. This means, again using Theorem 3.3.3, that the function in the integral above is in the Schwartz Space and is integrable(again see [15]).Therefore the integral will be finite and due to the extra $\frac{1}{N}$ factor the following holds

$$\mathrm{Var}_{\mu_N}\left(\frac{1}{N}\sum_{x\in\mathbb{Z}}\eta_{tN^2}(x,i)\phi(\frac{x}{N})\right)\underset{N\to\infty}{\to}0$$

3.3.3. Diffusive Case

In this section we investigate when the Freezing Model will show diffusive behaviour. To do this we can solve the PDE's of the system, equations (3.11). This is done by performing a Fourier-transform and subsequently a Laplace-transform to the equations. This method is further written out in section A.3 and results in the following PDE for the total density:

$$\begin{cases} \frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2} \\ \rho(x,0) = \tilde{\rho}(x) \end{cases} \tag{3.18}$$

where $D = \frac{1}{1+K}, K = \sum_{i=1}^{\infty} \frac{\gamma_i^u}{\gamma_i^d}$. To achieve the diffusive behaviour we must have that $K < \infty$.

Another way to find the PDE of the density is to note that the particles can only move in the ground layer. Therefor the Freezing Model will behave as a diffusive system consisting of random walkers, which scale to Brownian motion but with a scaled time to match the time that the particles in the Freezing Model spend in the ground layer. The fraction of the time the particles roam in the ground layer is exactly the stationary probability measure in layer 0, i.e. $\mu(0) = \lim_{N\to\infty} \mu_N(0)$. To find this $\mu(0)$ we will use the detailed balance equation (2.4) for the layers:

$$\mu(i)\gamma_i^d = \mu(0)\gamma_i^u$$

We know that the sum of all probabilities should be 1, i.e. $\sum_{i=0}^{\infty} \mu(i) = 1$. After some algebra the following can be obtained:

$$\mu(0) = \frac{1}{1 + \sum_{i=1}^{\infty} \frac{\gamma_i^d}{\gamma_i^u}}$$

which is exactly the diffusion constant D in (3.18) as expected.

3.3.4. Non-Diffusive Case

The diffusive character of the model only showed up if K was finite. This will not be the case if $K = \infty$ since there is no stationary distribution then in the ground layer, i.e. $\mu(0) = 0$. We can still use the equations (3.11) to find the PDE for this case.

Theorem 3.3.4 *Let $\tilde{\rho}_i \in C_b(\mathbb{R};\mathbb{R}_+)$ for $i \in \mathbb{N}_0$ be the initial density profiles of the layers and $(\mu_N)_{N\in\mathbb{N}}$ be a sequence of compatible initial conditions such that $\int \eta(y) d\mu_N = \rho(\frac{y}{N})$. Let $\mathbb{P}_{\mu_N}$ be the law of the measure valued-process:*

$$\{X^N(t) : t \geq 0\}, \qquad X^N(t) := (X^{i,N}(t))_{i\in\mathbb{N}_0} \tag{3.19}$$

Let $g \in C_c^\infty(\mathbb{R})$. Then $\forall\, T, \delta > 0$,

$$\lim_{N\to\infty} \mathbb{P}_{\mu_N}\left(\sup_{t\in[0,T]} \left| \langle X_t^{0,N}, g\rangle - \int_{\mathbb{R}} \rho_t(x,0) g(x) dx \right| > \delta \right) = 0 \tag{3.20}$$

where $\rho_t(x,0)$ solve the following PDE:

$$\begin{cases} \frac{\partial \rho_0(x,t)}{\partial t} = \Delta\rho_0(x,t) + D_t^{-\gamma}\rho_0(x,t) - C\rho_0(x,t) + \sum_{i=1}^{\infty} \gamma_i^d e^{-\gamma_i^d t}\tilde{\rho}_i(x) \\ \rho_0(x,0) = \tilde{\rho}_0(x) \end{cases} \tag{3.21}$$

where

$$D_t^{-\gamma} f(t) = \int_0^t \left(\sum_{i=1}^{\infty} \gamma_i^d \gamma_i^u e^{-\gamma_i^d (t-s)} \right) f(s) ds \tag{3.22}$$

Proof: Equation (3.20) is proven in Theorem 3.3.1. Note from (3.11) we get for each $i \geq 1$,

$$\rho_t(x,i) = e^{-\gamma_i^d t}\tilde{\rho}_i(x) + \int_0^t \gamma_i^d \gamma_i^u e^{-\gamma_i^d(t-s)}\rho_s(x,0) \tag{3.23}$$

Plugging this into (3.11) we get equation (3.21). □

We can analyse the non-diffusive case further by investigating in what way the particles will freeze, i.e. what kind of decay the fraction of time in the ground layer follows. We will first introduce a theorem that links behaviour of the Laplace transform of a function as $\lambda \to 0$ with the behaviour of the function as $t \to \infty$,

Theorem 3.3.5 ***(Karamata's Tauberian Theorem)*** *Let $f : [0,\infty) \to \mathbb{R}$ of bounded-variation and define*

$$\omega(\lambda) = \int_0^\infty e^{-\lambda t} df(t)$$

If $r \in \mathbb{R}_+$, then the following statements are equivalent:

- *(i) $\omega(\lambda) \sim C\lambda^{-r}$ as $\lambda \to 0$*
- *(ii) $f(t) \sim \frac{C}{\Gamma(r+1)} t^r$ as $t \to \infty$*

Proof: See [6] □

Using this theorem we will now show that the probability that the particle is in the ground layer will decay as $t \to \infty$.

Theorem 3.3.6 *Let $\mu(i), i \in \mathbb{N}_0$ be the probability measure on the layers of the Freezing Model. Assume $F(t) = \sum_{i\neq 0} \gamma_i^u \gamma_i^d e^{-\gamma_i^d t} \approx t^{-\beta}$, where $1 < \beta < 2$. If $K = \sum_{i=1}^\infty \frac{\gamma_i^u}{\gamma_i^d} = \infty$, then*

$$\mu_t(0) \sim C t^{\beta-2} \tag{3.24}$$

Proof: As only the layers are now important and not the position on the layers, we use the generator for the layer jump process,

$$\mathscr{L} f(i) = I(i=0) \sum_{j=1}^\infty \gamma_j^u (f(j) - f(0)) + I(i \neq 0)\gamma_i^d (f(0) - f(i))$$

Let's assume we start from i=0 and call $\mu_t(i)$ the probability that we are in layer i at time t. Then we have the following equations:

$$\begin{aligned} \mu_t'(i) &= \mu_t(0)\gamma_i^u - \mu_t(i)\gamma_i^d \quad , \text{i} \neq 0 \\ \mu_t'(0) &= \sum_{j\neq 0} \gamma_j^d \mu_t(j) - \mu_t(0) \sum_{j\neq 0} \gamma_j^u \end{aligned}$$

Set $M = \sum_{j\neq 0} \gamma_j^u < \infty$, else the second PDE would not be well-defined. Note that $\int_0^\infty F(t)dt = M$. By solving the first PDE we get

$$\mu_t(i) = \mu_0(i)e^{-\gamma_i^d t} + \int_0^t \gamma_i^u e^{-\gamma_i^d(t-s)}\mu_s(0)ds$$

and plugging this in into the second PDE

$$\mu_t'(0) = (F * \mu(0))(t) - M\mu_t(0) \tag{3.25}$$

where $*$ denotes convolution, i.e. $(f*g)(t) = \int_0^t f(t-s)g(s)ds$ and

$$F(t) = \sum_{j\neq 0} \gamma_j^u \gamma_i^d e^{-\gamma_i^d t}$$

Let $\hat{F}(\lambda) = \int_0^\infty F(t)e^{-\lambda t}dt$ denote the Laplace transform of F. Then $\hat{F}'(\lambda) = -\int_0^\infty tF(t)e^{-\lambda t}dt$ and is equal to the following: as $\lambda \to 0$

$$\hat{F}'(\lambda) = -\int_0^\infty tF(t)e^{-\lambda t}dt = C\int_0^\infty -e^{-\lambda t}d(t^{2-\beta}) \approx C\lambda^{-(2-\beta)}$$

where we used Karamata's Tauberian Theorem in the last step. We conclude thath

$$\hat{F}(\lambda) \approx C\lambda^{\beta-1} + C_0$$

where $C_0 = M$. We then use equation (3.25) to find the Laplace transform of $\mu_t(0)$, i.e. $\hat{\mu}(\lambda) = \int_0^\infty \mu_t(0)e^{-\lambda t}dt$,

$$\hat{\mu}(\lambda) = \frac{1}{\lambda + M - \hat{F}(\lambda)} \approx C\lambda^{1-\beta}$$

Then by another application of the Tauberian theorem we obtain

$$\mu_t(0) \approx Ct^{\beta-2}$$

as $t \to \infty$. □

Rescaled Brownian Motion and sub-diffusive behaviour

In the diffusive case the random walkers will perform Brownian motion in the limit as $N \to \infty$ where the amount of time the walker performs Brownian motion is equal to the part of the time the walker is in layer 0. This is exactly the probability that the walker is in layer 0, i.e. $\frac{\theta(t)}{t} \to \mu(0)$ where $\theta(t)$ is the amount of time the walker is in layer 0. So the following holds:

$$X_t^{\mathrm{FM}} = X_{\theta(t)}^{\mathrm{RW}} \simeq B(\theta(t)) = B(\mu(0)\,t) \tag{3.26}$$

and

$$\mathbb{E}\left((X_t^{\mathrm{FM}})^2\right) = \mu(0)\,t \tag{3.27}$$

In the non-diffusive case the fraction of time the particles will be in layer 0 goes to 0, i.e. $\frac{\theta(t)}{t} \to 0$. We know from earlier calculations that the probability that a particle will be in layer 0 behaves like equation (3.24). This means that:

$$X_t^{\mathrm{FM}} = X_{\theta(t)}^{\mathrm{RW}} \simeq B(\mu(0)_t\,t) = B(t^{\beta-1}) \tag{3.28}$$

and

$$\mathbb{E}\left((X_t^{\mathrm{FM}})^2\right) = \mu_t(0)\,t = t^{\beta-1} \tag{3.29}$$

with $1 < \beta < 2$. We can conclude that the variance of the position of the walker grows slower than linearly with the time. This is a consequence from the fact that the fraction of time the walker spends in the ground layer, in which it can move in the x-direction, decays to 0 for large t. Due to the variance growing slower than linearly with t, the system will display sub-diffusive behaviour.

4

Simulations

In this chapter the simulations of the Freezing Model are shown and discussed. The simulations are built in Python. The first idea on how to program a system with particles following Markovian dynamics was to take small time steps and check for each particle if they would jump and if so, where they would jump to. This asked for a lot of random numbers to be generated in each step and checking if these would be higher or lower than the exponential distribution for the jump times of their current site. Also each particles distribution would change if they switched between layers. This required a lot of bookkeeping.

To solve this problem, the jump times for each layer were calculated before hand. We know the jump times per layer are distributed according to (3.2). We can then generate the jump times by first uniformly generating random numbers between 0 and 1. Then we apply the inverse of the probability distribution function of the jump times to generate said jump times[17]. This is done a number of times for each layer and the generated jump times are stored in a library. For the bottom layer a number of random actions are then generated according to (3.1). This is not necessary for other layers since jumping to the bottom layer is the only action they can perform. The particles are then all placed on the origin at $t = 0$. Each particle will leap through time to their next jump time, randomly chosen from the set of already generated jump times for the layer that they are in. In this way the particles make bigger time steps, hopping through time from jump to jump, skipping the time steps where they do nothing and greatly reducing the computation time.

In the following figures the variance of the position of the particles is plotted against the time. We will compare this with the variance of a normal Brownian motion with diffusion constant equal to 2. The reason for this is the fact that we set the rates of going left or right equal to 1, which makes the total rate(and thus the diffusion constant) equal to 2. Additionally, a curvefit of the function $f(x) = ax^b$ is plotted of the variance of the particles in the Freezing Model. We will check if the variance of the particles positions follow equations (3.27 and (3.29) . We will mainly look at the power of t of the curvefit, because this tells us if the system shows diffusive or non-diffusive behaviour.

The system is first initiated with $\gamma_i^u = \frac{1}{i}$ and $\gamma_i^d = i$ with 1 layer and 50 layers. 2000 particles are placed in the system and the program runs for 10 seconds. Looking at the condition for diffusion in (3.18), we expect diffusion-like behaviour from this setup since $\sum_{i=1}^{\infty} \frac{\gamma_i^u}{\gamma_i^d} = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6} < \infty$. The variance of the particles position for the model with 1 layer is plotted in Figure 4.1 against the time, along with the variance of normal Brownian motion and the curvefit of the variance. The same is plotted in Figure 4.2 for 50 layers.

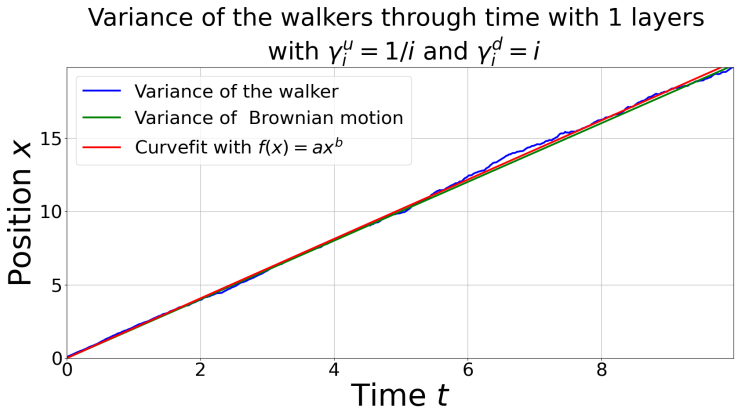

Figure 4.1: The variance of the position of the walkers in the Freezing Model with 1 layer plotted against the time where $\gamma_i^u = \frac{1}{i}$ and $\gamma_i^d = i$. The variance of the Brownian motion and the curvefit with $f(x) = ax^b$ are also plotted. The found values for the curvefit are a=2.041 $\pm$ 0.008and b=0.996 $\pm$ 0.002

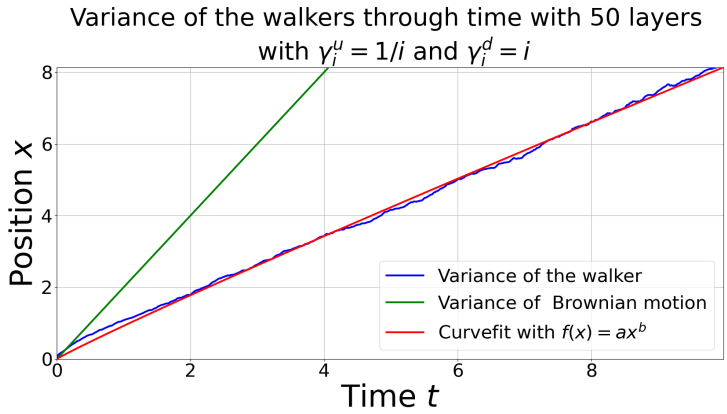

Figure 4.2: The variance of the position of the walkers in the Freezing Model with 50 layers plotted against the time where $\gamma_i^u = \frac{1}{i}$ and $\gamma_i^d = i$. The variance of the Brownian motion and the curvefit with $f(x) = ax^b$ are also plotted. The found values for the curvefit are a=0.924 $\pm$ 0.005and b=0.946$\pm$ 0.003

We can see that the variance of the particles position in the Freezing model with the aforementioned rates and consisting of 1 layer follows the variance of the Brownian motion closely. The curvefit returns a power of t of 0.996. This is close to 1, which is the power of t in the variance of Brownian motion. This is as expected since the model with 1 layer imitates particles performing a symmetric random walk on a one-dimensional integer line, which scales towards Brownian Motion. For 50 layers the curvefit returns a power of 0.946, which is a bit lower but still close to 1. Therefore, the model again exhibits Brownian-like motion as expected with these jump rates.

We now switch the rates to $\gamma_i^u = i$ and $\gamma_i^d = \frac{1}{i}$. Again looking at (3.18), this time the diffusion condition is not satisfied since $\sum_{i=1}^{\infty} \frac{\gamma_i^u}{\gamma_i^d} = \sum_{i=1}^{\infty} i^2 = \infty$. The program will run for 5 and 50 layers. Even though the sum of the ratio of the rates will be finite, we expect that as the number of layers increases, the behaviour of the system will become more and more sub-diffusive. The program is again run for 10 seconds with 2000 particles. The variance of the particles position for the model with 5 layer is plotted in Figure 4.3 against the time, along with the variance of normal Brownian motion and the curvefit of the variance. The same is plotted in Figure 4.4 for 50 layers without the variance of the Brownian motion.

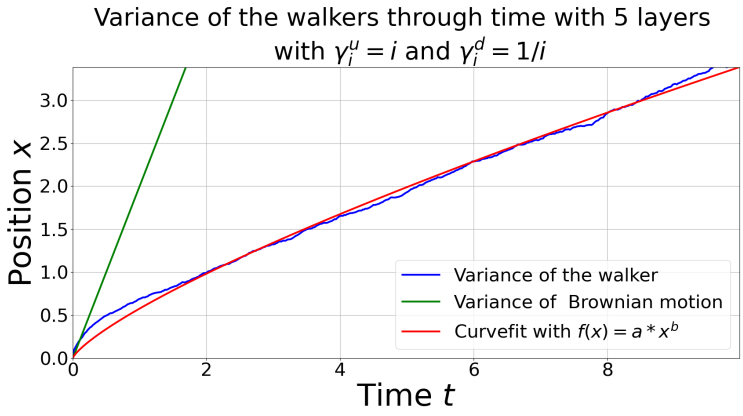

Figure 4.3: The variance of the position of the walkers in the Freezing Model with 50 layers plotted against the time where $\gamma_i^u = i$ and $\gamma_i^d = \frac{1}{i}$. The variance of the Brownian motion and the curvefit with $f(x) = ax^b$ are also plotted. The found values for the curvefit are a=0.576 ± 0.004and b=0.770± 0.003

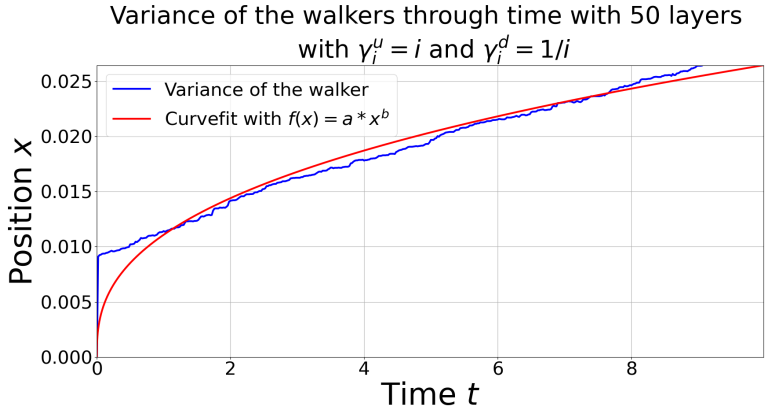

Figure 4.4: The variance of the position of the walkers in the Freezing Model with 50 layers plotted against the time where $\gamma_i^u = i$ and $\gamma_i^d = \frac{1}{i}$. The variance of the Brownian motion and the curvefit with $f(x) = ax^b$ are also plotted. The found values for the curvefit are a=0.011086 ± 0.00008and b=0.378± 0.004

With only 5 layers the curvefit already returns a power of t of 0.770, which is significantly smaller than 1. From the plot it is clear to see that the variance of the particles positions grows notably slower than t. For the instance with 50 layers this sub-diffusive behaviour is even more prominent, with the curvefit returning a power of 0.378 for the variance.

It is worth noting the difference between the diffusive and non-diffusive case. In the first model with 50 layers, the variance grew with $t^{0.946}$, where as in the second model the variance grew with $t^{0.378}$. This powers of t for both cases clearly show the difference between the diffusive and non-diffusive behaviour, depending on the jumping rates.

5

Concluding Remarks

The key thing to lay emphasis on is the difference in diffusive and non-diffusive behaviour of the Freezing Model. When the sum of the ratios of rates up divided by the rates down is finite, the model exhibits diffusive behaviour. The time the particles occupy the ground layer where they move diffusively grows linearly with t. This results in Brownian motion like movement. The density of the system then satisfies the heat equation with a diffusion constant involving the rates. When the aforementioned sum is infinite, the particles occupy the ground layer an amount of time that grows less than linear with t. For that reason they exhibit sub-diffusive behaviour. The PDE of the density now possesses a term that takes into consideration the past behaviour of the system. This *memory* aspect is worth noting, since we started off with a Markovian process, which is known for its memorylessness.

It is worth mentioning that the probability measures were not defined specifically, besides the fact that they are compatible with the initial conditions and that they are memoryless for the Markov property. An assumption for Poisson distributions as initial distributions would have made the calculations easier, but the result less general.

The Freezing Model contains a one-dimensional integer line with at each site per layer the same rates. For future research the model can be expanded into higher dimensions, modelling particles moving on surfaces or through volumes. Another interesting feature to add is different rates per site and see what kind of behaviour the model will exhibit then. This could imitate certain locations being colder than other ones, which causes the particles to have a higher chance to freeze there.

The goal of the simulations done in this thesis was to show that the model would exhibit diffusion-like behaviour or non-diffusive like behaviour depending on the rates. It was shown that for the non-diffusive case, the variance would grow significantly slower than linearly with t. However, the relation between the power of t with which the variance grows and the number of layers(and thus the diffusion constant) can still be further investigated.

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A

Appendix

A.1. Scaling Parameter

The process must be invariant under the scaling. This means the differential equation of the density must be invariant under scaling.

The equation is of the form:

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} \tag{A.1}$$

Now the following coordinate transformations are applied:

$$\begin{aligned} x' &= ax + x_0 \\ t' &= bt + t_0 \end{aligned} \tag{A.2}$$

Plugged into (A.1) gives:

$$b\frac{\partial \rho}{\partial t'} = a^2 D\frac{\partial^2 \rho}{\partial x'^2} \tag{A.3}$$

Since the equation is invariant under this scaling,

$$\frac{\partial \rho}{\partial t'} = D\frac{\partial^2 \rho}{\partial x'^2} \tag{A.4}$$

holds, which implies that $b = a^2$. In other words, a scaling by a factor a in space results in a scaling by a factor $b = a^2$ in time. In the model from this thesis space is scaled by a factor N, which implies that the time should be scaled by a factor N^2.

A.2. PDE Derivation

In this section we will derive the PDE's for the densities of the Freezing Model. We start with the generator of the model operating on a site in the configuration

$$\begin{aligned} \mathscr{L}\eta(x,i) = I(i=0)\left(\eta(x+1,i) - 2\eta(x,i) + \eta(x-1,i) + \sum_{n=1}^{\infty}\left(\gamma_n^d \eta(x,n) - \gamma_n^u \eta(x,i)\right)\right) \\ + I(i\neq 0)\left(\gamma_i^u \eta(x,0) - \gamma_i^d \eta(x,i)\right) \end{aligned} \tag{A.5}$$

Define the empirical density field as:

$$\pi_N(\eta) := \frac{1}{N}\sum_{x\in S}\eta_{tN^2}(x,i)\delta(\frac{x}{N},i) \tag{A.6}$$

Then:

$$\begin{aligned}
&\mathscr{L}^{(N)}\langle\pi_N(\eta),\phi\rangle = \\
&\quad\frac{1}{N}\sum_{x\in S}N^2\phi(\frac{x}{N},i)\left[I(i=0)\left(\eta(x+1,i)-2\eta(x,0)+\eta(x-1,0)+\sum_{n=1}^{\infty}\left(\frac{\gamma_n^d}{N^2}\eta(x,n)-\frac{\gamma_n^u}{N^2}\eta(x,i)\right)\right)\right. \\
&\qquad\left.+I(i\neq 0)\left(\frac{\gamma_i^u}{N^2}\eta(x,0)-\frac{\gamma_i^d}{N^2}\eta(x,i)\right)\right] \\
&=\frac{1}{N}\sum_{x\in S}N^2\eta(x,i)\left[I(i=0)\left(\phi(\frac{x+1}{N},i)-2\phi(\frac{x}{N},i)+\phi(\frac{x-1}{N},i)+\sum_{n=1}^{\infty}\left(\frac{\gamma_n^d}{N^2}\phi(\frac{x}{N},n)-\frac{\gamma_n^u}{N^2}\phi(\frac{x}{N},i)\right)\right)\right. \\
&\qquad\left.+I(i\neq 0)\left(\frac{\gamma_i^u}{N^2}\phi(\frac{x}{N},0)-\frac{\gamma_i^d}{N^2}\phi(\frac{x}{N},i)\right)\right] = (\square)
\end{aligned} \tag{A.7}$$

The offsets on the η's were moved to ϕ's and the parameters were rescaled by a factor of $\frac{1}{N^2}$. Note that:

$$\begin{aligned}
&\lim_{h\to 0}\frac{\phi(x+h)-2\phi(x)+\phi(x-h)}{h^2}=\phi''(x) \\
&\iff \\
&\lim_{N\to\infty}N^2\left(\phi(x+\frac{1}{N})-2\phi(x)+\phi(x-\frac{1}{N})\right)
\end{aligned} \tag{A.8}$$

Using then substitution $h=\frac{1}{N}$. Then equation (A.7) becomes as $N\to\infty$:

$$\begin{aligned}
(\square)\underset{N\to\infty}{\to}\frac{1}{N}\sum_{x\in S}\eta(x,i)\,[\,&I(i=0)\phi''(\frac{x}{N})+\sum_{n=1}^{\infty}\left(\gamma_n^d\phi(\frac{x}{N},n)-\gamma_n^u\phi(\frac{x}{N},i)\right) \\
&+\,I(i\neq 0)\left(\gamma_i^u\phi(\frac{x}{N},0)-\gamma_i^d\phi(\frac{x}{N},i)\right)\Big]
\end{aligned} \tag{A.9}$$

This is a simple Riemann sum and converges to the following integral:

$$\begin{cases}\int\left(\phi''(x,0)+\sum_{n=1}^{\infty}\left(\gamma_n^d\phi(x,n)-\gamma_i^u\phi(x,0)\right)\right)\rho(x,0)dx & \text{, for i=0}\\ \int\left(\gamma_i^u\phi(x,0)-\gamma_i^d\phi(x,i)\right)\rho(x,i)dx & \text{, for i}\neq 0\end{cases} \tag{A.10}$$

Thus the following PDE's are satisfied:

$$\begin{cases}\frac{\partial\rho_t(x,0)}{\partial t}=\Delta\rho_t(x,0)+\sum_{i\geq 1}\left(\gamma_i^d\rho_t(x,i)-\gamma_i^u\rho_t(x,0)\right)\\ \frac{\partial\rho_t(x,i)}{\partial t}=\gamma_i^u\rho_t(x,0)-\gamma_i^d\rho_t(x,i)\end{cases} \tag{A.11}$$

A.3. Solving PDE

Lets assume that all the particles start in the moving layer at t=0, i.e. $\tilde{\rho}_i(x)=0$ for i≥1. Then by applying a Fourier transform in x and a Laplace transform in t to equations (3.11) we get:

$$\begin{cases}\lambda\hat{\rho}_0(k,\lambda)-\tilde{\rho}_0(k)=-k^2\hat{\rho}_0(k,\lambda)+\sum_{i=1}^{\infty}\left[\gamma_i^d\hat{\rho}_i(k,\lambda)-\gamma_i^u\hat{\rho}_0(k,\lambda)\right]\\ \lambda\hat{\rho}_i(k,\lambda)=\gamma_i^u\hat{\rho}_0(k,\lambda)-\gamma_i^d\hat{\rho}_i(k,\lambda)\end{cases} \tag{A.12}$$

Where $\hat{\rho}_i(k,\lambda)$ is the Fourier- and Laplace-transform of $\rho_i(x,t)$ and $\tilde{\rho}_0(k)$ is the Fourier-transform of $\tilde{\rho}_0(x)$.

The second equation of (A.12) becomes:

$$\hat{\rho}_i(k,\lambda) = \frac{\gamma_i^u}{\lambda+\gamma_i^d}\hat{\rho}_0(k,\lambda) \tag{A.13}$$

Plugging this into the first equation of A.12 and simplifying:

$$\begin{aligned}\hat{\rho}_0(k,\lambda) &= \frac{\tilde{\rho}_0}{\lambda + k^2 + \sum_{i=1}^{\infty}(\gamma_i^u - \frac{\gamma_i^d\gamma_i^u}{\lambda+\gamma_i^d})} \\ &= \frac{\left(\prod_{i=1}^{\infty}(\lambda+\gamma_i^d)\right)\tilde{\rho}_0}{\left(\prod_{i=1}^{\infty}(\lambda+\gamma_i^d)\right)\left(\lambda+k^2+\sum_{i=1}^{\infty}\gamma_i^u\right) - \sum_{i=1}^{\infty}\gamma_i^d\gamma_i^u\prod_{\substack{i=1\\i\neq j}}^{\infty}(\lambda+\gamma_j^d)}\end{aligned} \tag{A.14}$$

Using equation (A.13) and adding all the layers up we get the following for the transform of the total density:

$$\hat{\rho}(k,\lambda) = \frac{\left[\left(\prod_{i=1}^{\infty}(\lambda+\gamma_i^d)\right) + \sum_{i=1}^{\infty}\gamma_i^u\left(\prod_{\substack{j=1\\j\neq i}}^{\infty}(\lambda+\gamma_i^d)\right)\right]\tilde{\rho}_0}{\left(\prod_{i=1}^{\infty}(\lambda+\gamma_i^d)\right)\left(\lambda+k^2+\sum_{i=1}^{\infty}\gamma_i^u\right) - \sum_{i=1}^{\infty}\gamma_i^d\gamma_i^u\prod_{\substack{i=1\\i\neq j}}^{\infty}(\lambda+\gamma_j^d)} \tag{A.15}$$

The diffusion, and thus the PDE of the total density ρ, is invariant under the rescaling of the space by a factor of $\frac{1}{N}$ and the time by a factor of N^2 as $N\to\infty$. This implies that the Fourier- and Laplace-transform should be invariant when k is rescaled by $\frac{1}{N}$ and λ is rescaled by $\frac{1}{N^2}$ since t and λ have inverse scalings([8]). Let $\epsilon = \frac{1}{N}$, then the following must hold:

$$\lim_{\epsilon\to 0}\epsilon^2\hat{\rho}(\epsilon k,\epsilon^2\lambda) = \hat{\rho}(k,\lambda) \tag{A.16}$$

Applying this limit to equation (A.15) we get:

$$\lim_{\epsilon\to 0}\epsilon^2\hat{\rho}(\epsilon k,\epsilon^2\lambda) = \frac{\left(\prod_{i=1}^{\infty}\gamma_i^d + \sum_{i=1}^{\infty}\gamma_i^u\prod_{\substack{j=1\\j\neq i}}^{\infty}\gamma_j^d\right)\tilde{\rho}_0}{\left(\prod_{i=1}^{\infty}\gamma_i^d + \sum_{i=1}^{\infty}\gamma_i^u\prod_{\substack{j=1\\j\neq i}}^{\infty}\gamma_j^d\right)\lambda + \left(\prod_{i=1}^{\infty}\gamma_i^d\right)k^2} \tag{A.17}$$

Dividing numerator and denominator by $\prod_{i=1}^{\infty}\gamma_i^d$ we get:

$$\hat{\rho}(k,\lambda) = \frac{\left(1+\sum_{i=1}^{\infty}\frac{\gamma_i^u}{\gamma_i^d}\right)\tilde{\rho}_0}{\left(1+\sum_{i=1}^{\infty}\frac{\gamma_i^u}{\gamma_i^d}\right)\lambda + k^2} \tag{A.18}$$

or:

$$\hat{\rho}(k,\lambda) = \frac{\hat{\rho}_0}{\lambda + Dk^2} \tag{A.19}$$

where $D = \frac{1}{1+\sum_{i=1}^{\infty}\frac{\gamma_i^u}{\gamma_i^d}}$.

This is exactly the Fourier- and Laplace-transform we get from the following PDE:

$$\frac{\partial\rho}{\partial t} = D\frac{\partial^2\rho}{\partial x^2} \tag{A.20}$$

with initial condition $\rho(x,0) = \rho_0$. Since the Fourier-transform and the Laplace-transform are unique, the density profile of the Freezing Model follows equation (A.20) if $\sum_{i=1}^{\infty}\frac{\gamma_i^u}{\gamma_i^d} < \infty$.

A.4. Duality for two particles

For convenience the theorem is repeated:

Let $\{X_t : t \geq 0\}$ *and* $\{Y_t : t \geq 0\}$ *be two random walkers in the Freezing Model. Then the following dual duality holds:*

$$\mathbb{E}_\eta \left[\frac{\eta_t(x,i)}{\alpha_i} \frac{\eta_t(y,j)}{\alpha_j} \right] = \mathbb{E}^{\text{RW's}}_{((x,i),(y,j))} \left[\frac{\eta(X_t,i_t)}{\alpha_{i_t}} \frac{\eta(Y_t,j_t)}{\alpha_{j_t}} \right] \tag{A.21}$$

Proof:

$$\begin{aligned}
\mathbb{E}_\eta \left[\frac{\eta_t(x,i)}{\alpha_i} \frac{\eta_t(y,j)}{\alpha_j} \right] &= \mathbb{E} \left[\left(\sum_{(x',i')} \sum_{k=1}^{\eta(x',i')} I(X_t^{k,(x',i')} = (x,i)) \frac{1}{\alpha_i} \right) \right. \\
&\qquad \left. \left(\sum_{(y',j')\neq(x',i')} \sum_{n=1}^{\eta(y',j')} I(Y_t^{n,(y',j')} = (y,j)) \frac{1}{\alpha_j} + \sum_{n\neq k} I(Y_t^{n,(x',i')} = (y,j)) \frac{1}{\alpha_j} \right) \right] \\
&= \mathbb{E} \left[\sum_{(x,i')} \sum_{(y',j')\neq(x',i')} \sum_{k=1}^{\eta(x',i')} \sum_{n=1}^{\eta(y',j')} I(X_t^{k,(x',i')} = (x,i)) I(Y_t^{n,(y',j')} = (y,j)) \frac{1}{\alpha_i} \frac{1}{\alpha_j} \right. \\
&\qquad \left. + \sum_{(x,i')} \sum_{k=1}^{\eta(x',i')} \sum_{n\neq k} I(X_t^{k,(x',i')} = (x,i)) I(Y_t^{n,(x',i')} = (y,j)) \frac{1}{\alpha_i} \frac{1}{\alpha_j} \right] \\
&= \sum_{(x',i')} \sum_{(y',j')\neq(x',i')} \eta(x',i')\eta(y',j') P_t((x',i'),(x,i)) P_t((y',j'),(y,j)) \frac{1}{\alpha_i} \frac{1}{\alpha_j} \\
&\qquad + \sum_{(x',i')} \eta(x',i')(\eta(x',i')-1) P_t((x',i'),(x,i)) P_t((x',i'),(y,j)) \frac{1}{\alpha_i} \frac{1}{\alpha_j} \\
&= \sum_{(x',i')} \sum_{(y',j')} \eta(x',i')\eta(y',j') P_t((x,i),(x',i')) P_t((y,j),(y',j')) \frac{1}{\alpha_i} \frac{1}{\alpha_{j'}} \\
&\qquad - \sum_{(x',i')} \eta(x',i') P_t((x,i),(x',i')) P_t((y,j),(x',i')) \frac{1}{\alpha_{i'}^2} \\
&= \mathbb{E}^{\text{RW's}}_{((x,i),(y,j))} \left[\frac{\eta(X_t,i_t)}{\alpha_{i_t}} \frac{\eta(Y_t,j_t)}{\alpha_{j_t}} \right] - \sum_{(x',i')} \eta(x',i') P_t((x,i),(x',i')) P_t((y,j),(x',i')) \frac{1}{\alpha_{i'}^2}
\end{aligned}$$

where we used $\mathbb{E}\left[I(X_t^{(z,l)} = (x,i)) I(Y_t^{(r,m)} = (y,j)) \right] = P_t^{(2)}((z,l),(x,i);(r,m),(y,j)) = P_t((x',i'),(x,i)) P_t((y',j'),(y,j))$ in the third equality using the independence of the random walkers. In the fourth equality the detailed balance equation was used for both random walkers.

A.5. Python Code

Listed below is the Python code used to model the Freezing model for the non-diffusive case. The diffusive case can be obtained by switching the functions for the rates.

```
import random
import numpy as np
import math
import matplotlib.pyplot as plt
import scipy.stats
import time
from numba import jit
from scipy.optimize import curve_fit

#define jump rates and jump time distributions
```

```
def g_u(n):
    return n**0.5


def g_d(n):
    return 1/n**0.5

def inv_exp(l, x):
    return -1/l*np.log(1-x)


start_time = time.time()


N=5

layers = [0, 4]

for m in layers:
    nr_actions = 100000
    x = np.array([random.random() for i in range(nr_actions)])
    x_0 = np.array([random.random() for i in range(nr_actions*10)])


    #Calculate jump times
    jump_times = {}
    jump_times['0'] = list(inv_exp(2+sum(g_u(j)/N**2 for j in range(1, m)), x_0))
    for j in range(1, m):
        jump_times[str(j)] = list(inv_exp(g_d(j)/N**2, x))


    #Calculate actions on layer 0
    z = [random.uniform(0, 2+sum(g_u(j)/N**2 for j in range(1, m))) for n in range(len(x)*1
    action_0 = ['left' if i<=1 else 'right' if (1<=i and i<=2) else i-2 for i in z]


    for i in range(len(action_0)):
        if isinstance(action_0[i], float):
            s=action_0[i]
            n=0
            while s>0:
                n+=1
                s-=g_u(n)/N**2
            action_0[i] = n

    print('time after calculating jump_times and actions: ', time.time()-start_time)

    #Initiate particles with [x_positionm, layer, time]
    nr_particles = 1000
```

```
end_time = 10*N**2
final_locs = []
for k in range(nr_particles):
    locs = [[0, 0, 0]]
    inter_loc = [[0, 0, 0], jump_times['0'].pop()]
    while locs[-1][2] < end_time:
        inter_loc[0][2] += inter_loc[1]
        if inter_loc[0][1] == 0:
            action = action_0.pop()
            if action == 'left':
                inter_loc[0][0] -= 1/N
                inter_loc[1] = jump_times['0'].pop()
            elif action == 'right':
                inter_loc[0][0] += 1/N
                inter_loc[1] = jump_times['0'].pop()
            else:
                inter_loc[0][1] += action
                inter_loc[1] = jump_times[str(action)].pop()
        else:
            inter_loc[0][1] = 0
            inter_loc[1] = jump_times['0'].pop()
        locs.append(inter_loc[0].copy())
    final_locs.append(locs)


print('Time after calculating walks: ', time.time()-start_time)

#sort the particles positions per time step
dt = 0.5
inter_t = dt
min_locs = [[final_locs[i][0][0]] for i in range(len(final_locs))]


while inter_t < end_time:
    inter_t += dt
    next_locs = [[final_locs[i][j][0] for j in range(len(final_locs[i])) if final_locs[
    min_locs = [min_locs[i] + [next_locs[i][0]] for i in range(len(min_locs))]

#calculate variance of particles
var_x = np.array([np.var([min_locs[i][j] for i in range(len(min_locs))]) for j in range
t = np.array([i*dt for i in range(len(var_x))])


#plot the variance and the variance of normal Brownian motion
plt.figure()
plt.plot(t/N**2, var_x, label = 'Variance of the walker', c='b', lw = 3)
if m==0 or m==4:
    plt.plot(t/N**2, 2*t/N**2, label = 'Variance of  Brownian motion', c='g', lw = 3)
plt.title('Variance of the walkers in the Freezing Model through time with {} layers\n
```

```
print('Time after variance: ', time.time()-start_time)

#calculate curve_fit
def func(x, a, b):
    return a*x**b

popt, pcov = curve_fit(func, t/N**2, var_x)
t_0 = np.linspace(0, max(t/N**2), 10000)
print(popt)

#plot curve_fit
plt.plot(t_0, func(t_0, *popt), label = 'Curvefit with $f(x)=a*x^{b}$', c='r', lw = 3)
plt.legend(fontsize ='30')
plt.xlabel('Time $t$', fontsize ='50')
plt.ylabel('Position $x$', fontsize ='50')
plt.grid(True)
plt.xlim(0, max(t/N**2))
plt.ylim(0, min([var_x[-1], func(t_0[-1], *popt)]))
plt.tick_params(labelsize ='30')
plt.show()
```