Hydrodynamic limits for the exclusion process with disorder and reservoirs

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1 Introduction

Interacting particle systems are classical models to study problems in non-equilibrium statistical physics. For instance, interacting particle systems can be used successfully to derive Fourier's law, on heat conduction. Furthermore, interacting particle systems have been used to prove new theorems in non-equilibrium statistical physics, such as the fluctuation theorem [4].A typical example of these interacting particle systems is the symmetric exclusion process (SEP)[8]. While these interacting particle systems will always fall short capturing the full complexity of physical reality, they still enable us derive essential characteristics of it, through a rigorous mathematical approach. The SEP is a stochastic process that describes particles hopping randomly on a grid of sites. The most simple case of the SEP follows two key rules. First that no two particles can occupy the same site. This explains the "exclusion" part in its name. The second rule being that the jumps to the neighbouring sites on the left and right occur with equal probability. This explains the "symmetric" part in the name. There are various types of SEPs, with different modelling restriction, including some that are exceptions to the two key rules mentioned above. In this thesis four different types of SEPs have been considered.

Starting from these four SEPs, the goal of this thesis is to show that the mathematical approach of duality can be used to prove the time evolution of the collective behaviour of the particles under consideration. Duality is a mathematical technique to relate the properties of one type of model to the properties of another one [2]. The duality approach allows us to reduce a system with possibly infinitely many particles to a system with a finite number of particles, up to even only one particle. This enables substantial computational simplification. Moreover, duality makes it possible to replace a boundary site, where particles can enter and leave the system, by an absorbing site where particles can only leave the system[1]. This also adds to further simplification of the model.The time evolution of the collective behaviour of the particles is characterized by the hydrodynamic limit. The hydrodynamic limit describes the mathematical method to move from a microscopic to a macroscopic perspective. The aim is to show that this result can be achieved through the use of duality. Using duality will make the proof much more intuitive than the elaborate approach used in [3] and [6]. Furthermore, it will allow us to create proofs for systems that so far have been proven by such another and more elaborate approach.

On this basis, the approach that is taken during the project is as follows. First we consider the SEP on the homogeneous environment $\mathbb{F}$. This model does not allow particles to enter or leave the system and only allows for one particle per site. Using duality the problem is reduced to a single-particle problem and after diffusive scaling leads to the expected result: the solution to the heat equation. Diffusive scaling is accomplished by introducing the scaling factor N and scaling space by $\frac{1}{N}$ and time by N^2.

In the next model we allow for more particles to occupy the same site, thus relaxing one of the key rules for SEPs mentioned above. In this model we still make use of diffusive scaling. Using duality, we once again reduce the problem to a single-particle problem. Furthermore, we apply an important result derived from the study of the random conductance model (RCM), to obtain the desired result: the solution to the heat equation, with a diffusion coefficient that depends on the maximum occupancy of the sites.

In the third model we assume an open system and allow particles to enter and leave the system at the left and right boundary sites. The rates at which particles can enter and leave the system are set by certain parameters. However, in this model the maximum occupancy of the sites is again 1, as it was in the first model. Now we use duality to relate the model to a single-particle model where the boundary sites (where particles can both enter and leave) are replaced by absorbing sites (where particles can only leave). After applying diffusive scaling once again, we obtain the expected result: the solution of the heat equation with Dirichlet boundary values, depending on the parameters describing exchange rates at the boundary sites.

In the fourth, and final model, the properties of the second and third model were combined. Thus, an open system is studied, where more than one particle can occupy the same site. In order to prove the expected outcome, the results from the second and third model are combined. The resulting outcome is the heat equation with Dirichlet boundary values depending on the behaviour at the boundaries and a diffusion coefficient depending on the random environment.

Lastly, a physical application is discussed to illustrate how the theoretical results obtained from the analysis of SEPs can be used to better understand real-world phenomena. In particular, we consider the migration of Li^+ ions through the electrolyte of a lithium battery. the migration of these ions can be modelled by the $\text{SEP}^{L,R}$ and $\text{SEP}^{L,R}(\boldsymbol{\alpha})$, depending on the disorder the anion sublattice. The derived hydrodynamic limits provide insight into how microscopic disorder in the electrolyte influences ionic conductivity, and hence the performance of the battery. This example not only demonstrates not only demonstrates the practical relevance of interacting particle systems, but also shows how mathematics and physics can complement each other.

In conclusion, this project demonstrates the feasibility of using duality to derive the hydrodynamic limit of given SEPs. In particular it shows how duality can be used to derive the hydrodynamic limit of a open systems with a random maximum occupancy. For this model a proof had not been available yet. Furthermore, by applying these results to a physical system, namely the migration of Li^+ ions in lithium batteries, this thesis illustrates how interacting particle systems can be used to understand and improve real-world technological processes.

2 Mathematical background

In this chapter, we will first provide the mathematical background needed to understand this thesis.

2.1 Markov theory

2.1.1 The Markov property

A Markov process on the state space Ω is a stochastic process $X_t, t \geq 0$, such that future states only depend on the current state and not on any past states. Mathematically, this is expressed as follows.

Definition 2.1 (the Markov property)**.** For all $t > 0$, $n \in \mathbb{N}$, $0 < t_1 < t_2 < ...t_n < t$ and for all $f : \Omega \to \mathbb{R}$ bounded and measurable, we have that

$$\mathbb{E}(f(X_t)|X_{t_1}, X_{t_2}, ..., X_{t_n}) = \mathbb{E}(f(X_t)|f(X_{t_n}) \tag{1}$$

Or in a more measure theoretic notation, which is also more useful for the continuous time case

Definition 2.2 (the Markov property measure theoretic notation)**.** Let $\mathcal{F}_t = \sigma(X_r : r \leq t)$ be the σ-algebra generated by the random variables $X_r, r \leq t$, then for all $0 < s \leq t$ it holds that

$$\mathbb{E}((f(X_t)|\mathcal{F}_s) = \mathbb{E}(f(X_t)|X_s)$$

2.1.2 Semigroups and generators

Definition 2.3 (Semigroup)**.** Let $\{X_t, t \geq 0\}$ be a Markov process on the state space Ω, then we define the semigroup S_t for a bounded function $f : \Omega \to \mathbb{R}$ as

$$S_t f(x) = \mathbb{E}(f(X_t)|X_0 = x) = \mathbb{E}_x(f(X_t)) \tag{2}$$

where $\mathbb{E}_x$ denotes the expectation of the process starting from $x \in \Omega$.

We prefer to think of S_t as an operator working on functions $f \in \mathcal{B}(\Omega)$. The most import properties of S_t are summarized in Proposition 2.1.

Proposition 2.1 (Properties of the Semigroup S_t).

1. *Identity at time zero:* $S_0 = I$, i.e., $S_0 f = f$ for all f.
2. *Right continuity:* The map $t \mapsto S_t f$ is right-continuous.
3. *Semigroup property:* For all $t, s \geq 0$,
$$S_{t+s} f = S_t(S_s f) = S_s(S_t f).$$
4. *Positivity:* If $f \geq 0$, then $S_t f \geq 0$.

5. *Normalization:* $S_t\mathbf{1} = \mathbf{1}$.

6. *Contraction:*
$$\sup_x |(S_t f)(x)| \leq \sup_x |f(x)|.$$

There is a one-to-one correspondence between a Markov generator $\mathcal{L}$ and a Markov semigroup $\{S_t, t \geq 0\}$ [8]

Definition 2.4. For all $f \in D(\mathcal{L})$, the generator $\mathcal{L}$ of the Markov process $\{X_t, t \geq 0\}$ is defined as
$$\mathcal{L}f = \lim_{t \to 0} \frac{S_t f - f}{t} \tag{3}$$
where the domain $D(\mathcal{L})$ is given by
$$D(\mathcal{L}) = \{f : \lim_{t \to 0} \frac{S_t f - f}{t} \quad \text{exists}\} \tag{4}$$

Notice that $\mathcal{L}$ is only defined for a much more restrictive class of functions, compared to the set of functions on which the semigroup can be defined.

2.2 Duality

Duality describes how two Markov processes $\{X_t, t \geq 0\}$ (the process under study) on a state space Ω and a process $\{Y_t, t \geq 0\}$ (the dual process) on a state space $\hat{\Omega}$ can be related to each other using a duality function $D : \hat{\Omega} \times \Omega \mapsto \mathbb{R}$. The relation between the Markov processes is expressed through expectations, i.e. for all $t \geq 0$ and for all $y \in \hat{\Omega}, x \in \Omega$
$$\hat{\mathbb{E}}_y(D(Y(t), x) = \mathbb{E}_x(D(y, X(t)). \tag{5}$$

We write the connection symbolically as
$$\{X_t, t \geq 0\} \overset{D}{\to} \{Y_t, t \geq 0\} \tag{6}$$

The main reason for looking for duality, (i.e. a dual process and a dual function) is simplification. In the context of interacting particles, one of the most important simplifications induced by duality is that it allows us to reduce systems with possibly infinitely many particles to systems with a finite number of particles. If we study interacting particle systems, which at the boundaries allow input and output of particles, duality allows us to connect the system to a much simpler system where the boundaries are replaced by absorbing sites.

2.2.1 Generator and semigroup duality

The relation introduced in 5 can be replaced by a similar relation between the Markov generators of the two processes. Since the Markov generator fully encodes the Markov process, in most cases, a duality relation for expectations

is derived from a duality relation between the generators.
We denote the semigroup of the process $\{X_t, t \geq 0\}$ by

$$(S_X(t)f)(x) = \mathbb{E}_x[f(X(t))], \tag{7}$$

and similarly $(S_Y(t)f)(x) = \mathbb{E}_y[f(Y(t))]$. We define the notion of semigroup duality in the following way.

Definition 2.5. Let $D : \hat{\Omega} \times \Omega \mapsto \mathbb{R}$ denote a measurable function. We say that D is a duality function for semigroup duality between the process $\{X_t : t \geq 0\}$ and the dual process $\{Y_t : t \geq 0\}$ if for all $x \in \Omega, y \in \hat{\Omega}$ and $t \geq 0$ we have

$$\hat{\mathbb{E}}_y(D(Y(t), x) = \mathbb{E}_x(D(y, X(t))), \tag{8}$$

The notion of semigroup duality in 8 is equivalent to the notion of "duality" given in eq. **??**. As a concise notation for semigroup duality we will write

$$\{X_t, t \geq 0\} \overset{D}{\to} \{Y_t, t \geq 0\} \tag{9}$$

Let $\mathcal{L}_X$ and $\mathcal{L}_Y$ denote the Markov generators of $\{X_t : t \geq 0\}$ and $\{Y_t : t \geq 0\}$ respectively. Then we say that the dual function $D(y, \cdot)$ is in the domain of the generator if

$$\mathcal{L}_X D(y, x) = \lim_{t \to 0} \frac{\mathbb{E}_x[D(y, X(t)] - D(y, x)}{t} \quad \text{exists for all } x \in \Omega \tag{10}$$

The same holds for $\mathcal{L}_Y$.
In case the duality functions are in the domain of the generator, we have the notation of "generator duality", which is defined as follows.

Definition 2.6. Let $D : \hat{\Omega} \times \Omega \mapsto \mathbb{R}$ be a function such that $D(y, \cdot)$ is in the domain of $\mathcal{L}_X$ and $D(\cdot, x)$ is in the domain of $\mathcal{L}_Y$. We then say that D is a duality function for generator duality between the process $\{X_t, t \geq 0\}$ and the dual process $\{Y_t, t \geq 0\}$ if for all $x \in \Omega, y \in \hat{\Omega}$ we have

$$(\mathcal{L}_Y D(\cdot, x))(y) = (\mathcal{L}_X D(y, \cdot))(x) \tag{11}$$

In case the state spaces Ω and $\hat{\Omega}$ are finite, the Markov generators are matrices. Because the semigroups are simply the matrix exponentials

$$S_X(t) = \sum_{n=0}^{\infty} \frac{t^n L_X^n}{n!} \tag{12}$$

and similarly $S_Y(t) = \sum_{n=0}^{\infty} \frac{t^n L_Y^n}{n!}$ we obtain semigroup duality from generator duality. However subtleties start to arise when the state spaces are no longer finite and the Markov generators become unbounded operators. The following theorem tells us when generator duality implies semigroup duality.

Theorem 2.7 (Relation between semigroup duality and generator duality [2])**.** *Let $\mathcal{L}_X$ denote the generator of the Markov process $\{X_t, t \geq 0\}$ and $\mathcal{L}_Y$ the generator of the Markov process $\{Y_t, t \geq 0\}$. Let $D : \hat{\Omega} \times \Omega \mapsto \mathbb{R}$ be a function such that $D(y, \cdot)$ is in the domain of $\mathcal{L}_X$ and $D(\cdot, x)$ is in the domain of $\mathcal{L}_Y$. If $(S_Y(t) \otimes I)D \in \mathcal{D}_X$ and $(I \otimes S_X(t))D \in \mathcal{D}_Y$ for all $t \geq 0$, then generator duality implies semigroup duality.*

Proof. For the proof we refer to [2] □

2.3 Brownian motion and the connection to the heat equation

First we state the definition of Brownian motion.

Definition 2.8 (Brownian motion)**.** A real valued process $\{W_t, t \geq 0\}$ is called a Brownian motion process if

1. *Starting at 0:* $W(0) = 0$.
2. *Normally distributed increments:* For all $0 \leq s \leq t$, $W(t) - W(s) \stackrel{d}{=} \mathcal{N}(0, t - s)$.
3. *Independent increments:* For all $0 \leq t_0 < t_1 < t_2 < .... < t_n$, the random variables $Y_i := W(t_i) - W(t_{i-1}), i = 1, ...n$ are independent.
4. *Continuous trajectories:* The map $t \mapsto W(t)$ is continuous.

Brownian motion is a Markov process. The Markov property can be verified using the independent increments of Brownian motion. For the exact proof we refer to [9]. We define the Markov semigroup of the Brownian motion process $W(t)$ as

$$S_t f(x) = \mathbb{E}_x[f(W(t))] = \mathbb{E}[f(x + W(t))] \tag{13}$$

The Markov generator of Brownian motion is formalized in Lemma 2.9

Lemma 2.9 (Markov generator of Brownian motion)**.** *For all $f \in \mathcal{C}_0^2(\mathbb{R})$, the Markov generator $\mathcal{L}$ of the Brownian motion process$\{W(t), t \geq 0\}$ is given by*

$$\mathcal{L}f(x) = \frac{1}{2} f''(x) \tag{14}$$

Proof. By Definition 2.4 we know that

$$\mathcal{L}f(x) = \lim_{t \to 0} \frac{S_t f(x) - f(x)}{t} = \lim_{t \to 0} \frac{\mathbb{E}[f(x + W(t))] - f(x)}{t} \tag{15}$$

If we then use property 2 of Definition 2.8 we find:

$$\mathcal{L}f(x) = \lim_{t \to 0} \frac{\int_{\mathbb{R}} f(z) \frac{1}{\sqrt{2\pi t}} e^{-\frac{(z-x)^2}{2t}} dz - f(x)}{t} \tag{16}$$

next we expand $f(z)$ in a Taylor expansion around x

$$f(z) = f(x) + f'(x)(z-x) + \frac{f''(x)(z-x)^2}{2!} + R_3(z) \tag{17}$$

plugging this back into the integral expression leads to

$$\mathcal{L}f(x) = \lim_{t\to 0} \frac{f(x) + \frac{1}{2}f''(x)t + o(t) - f(x)}{t} = \frac{1}{2}f''(x) \tag{18}$$

□

The heat equation is a partial differential equation that models the diffusion of particles in a given space over time:

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} \tag{19}$$

where $\rho(x,t)$ is the density of particles at time t and position x and D is the diffusion coefficient.
The solution to the heat equation can be interpreted as the probability density function of the position of a particle following Brownian motion. This is formalized in the following theorem.

Theorem 2.10 (Brownian motion and the heat equation [9])**.** *Let f be a bounded function. Then the unique solution of*

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2}$$

given by

$$\rho(x,t) = \mathbb{E}(f(B(2Dt) + x)$$

Proof. For the proof recall that the function

$$G(t,x,y) = \frac{e^{-\frac{(y-x)^2}{2t}}}{\sqrt{2\pi t}}$$

is the fundamental solution to the heat equation. That is

$$\rho(t,x) = \int G(t,x,y)\rho(0,y)dy$$

is the solution to the heat equation with initial condition $\rho(0,\cdot)$ □

2.4 Brownian motion with absorption sites

Next we consider a Brownian motion process with absorption sites $\{W_t^{abs}, t \geq 0\}$ on the interval $[0,1]$. The process starts at some point in the interval $[0,1]$ and evolves like standard Brownian motion until it reaches one of the absorption

sites 0 and 1. At that moment the process stops and sets to 0. If we let $\tau = \inf\{t > 0 | W_t^{abs} \notin (0,1)\}$ then

$$W_t^{abs} = \begin{cases} W(t) & t \leq \tau \\ 0 \text{ (absorbed)} & t \geq \tau \end{cases} \tag{20}$$

The behaviour of the absorbed Brownian motion on the interval $(0,1)$ is the same as the regular Brownian motion process and doesn't change after being absorbed. So, the generator of the absorbed Brownian motion process $\{W_t^{abs}, t \geq 0\}$ is given by

$$\mathcal{L}f(x) = \begin{cases} f''(x) & x \in (0,1) \\ 0 & x = 0, 1 \end{cases} \tag{21}$$

For all $f \in \mathcal{C}^2([0,1])$ the absorbed Brownian motion process is the solution to the heat equation with Dirichlet boundary conditions. This is formalized in Theorem 2.11

Theorem 2.11 (Absorbing Brownian motion and the heat equation)**.** *Let $f \in \mathcal{C}^2([0,1])$ with $f(0) = \rho_L$ and $f(1) = \rho_R$. Then the unique solution of*

$$\begin{aligned} \frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} \quad & x \in (0,1) \\ \rho(0,t) &= \rho_L \\ \rho(1,t) &= \rho_R \end{aligned} \tag{22}$$

given by

$$\rho(x,t) = \mathbb{E}(f(W^{abs}(2Dt) + x) \tag{23}$$

3 Symmetric exclusion process on a homogeneous environment

3.1 Model

Let us introduce the one-dimensional symmetric exclusion process in the homogeneous environment $\mathbb{Z}$, abbreviated by SEP, consisting of a collection of occupation variables indexed by the sites of $\mathbb{Z}$. These variables indicate the number of particles at each site, i.e.,

$$\eta_x := \text{the number of particles at site } x \tag{24}$$

Since each site can hold at most one particle, $\eta_x \in \{0,1\}$ for all $x \in \mathbb{Z}$, we define the configuration space χ as

$$\chi := \prod_{x\in\mathbb{Z}} \{0,1\} \tag{25}$$

The SEP is the Markov process on χ whose generator acts on bounded functions $f : \chi \to \mathbb{R}$, as follows

$$\mathcal{L}f(\eta) = \sum_{x\in\mathbb{Z}} \Big[\eta_x(1-\eta_{x+1})\big(f(\eta^{x,x+1}) - f(\eta)\big) + \eta_{x+1}(1-\eta_x)\big(f(\eta^{x+1,x}) - f(\eta)\big)\Big] \tag{26}$$

In the above formula $\eta^{x,x+1}$ denotes the configuration obtained from η by removing the particle (if any) form the site x and adding the particle to the site $x+1$, i.e.

$$\eta^{x,x+1} = \begin{cases} \eta - \delta_x + \delta_{x+1} & \text{if } \eta_x = 1 \text{ and } \eta_{x+1} = 0 \\ \eta & \text{otherwise} \end{cases} \tag{27}$$

So the rate to jump from site x to site $x+1$ is determined by the available sites at $x+1$ (i.e., $(1-\eta_{x+1})$) and the number of particles at site x (i.e., η_x).

3.2 Self-duality of the SEP

The SEP is a self-dual Markov process. This means that there exists a function $D : \chi_f \times \chi \to \mathbb{R}$ (with χ_f being a subset of configurations in χ), called the self-duality function, such that

$$\mathcal{L}D(\cdot,\eta)(\xi) = \mathcal{L}D(\xi,\cdot)(\eta) \tag{28}$$

for all $\xi \in \chi_f$ and $\eta \in \chi$. In particular, the l.h.s. corresponds to applying the generator $\mathcal{L}$ to the function $D(\cdot,\eta)$ and evaluating the resulting function at ξ, while the r.h.s corresponds to applying the generator to the function $D(\xi,\cdot)$ and evaluating the result at η. This self-duality property is formalized in Lemma 3.1.

Lemma 3.1 (Duality relation of the SEP)**.** *The symmetric exclusion process on the homogenous environment $\mathbb{Z}$, is a self-dual Markov process with self-duality function $D : \chi_f \times \chi \to \mathbb{R}$, given by*

$$D(\xi, \eta) := \prod_{x \in \mathbb{Z}} \frac{\binom{\eta_x}{\xi_x}}{\binom{1}{\xi_x}} \tag{29}$$

Since $\eta, \xi \in \{0,1\}^{\mathbb{Z}}$ this reduces to

$$D(\xi, \eta) = \prod_{x \in \mathbb{Z}} \mathbf{1}_{\{\xi_x \leq \eta_x\}} \tag{30}$$

Proof. See the Appendix □

We are interested in a particular instance of this self-duality property, namely when the dual configuration consists of a single particle, i.e. $\xi = \delta_x$ for some $x \in \mathbb{Z}$. If there is only one particle in the system, no interaction takes place and we are left with a single random walk, abbreviated by RW. In this case the duality function reduces to

$$D(\delta_x, \eta) = \eta_x \tag{31}$$

In this case we can conclude the following semigroup duality relation

$$\mathbb{E}_\eta^{SEP}\left(\eta_x(t)\right) = \mathbb{E}_x^{RW}\left(\eta_{x(t)}(0)\right) \tag{32}$$

3.3 Hydrodynamic limit of the SEP

In order to describe the macroscopic behaviour of the interacting particle system we want to make a transition from a micro to a macro perspective. In order to do so, we introduce a "scaling parameter" N, which has to be thought of as the ratio between the macroscopic and microscopic length scale. To the macropoint $x \in \mathbb{R}$ corresponds the micropoint $[Nx]$. We view a configuration of the exclusion process on a grid with spacing $\frac{1}{N}$. When N becomes large, rather than seeing all microscopic details of which sites are occupied and which are not, we see the "density profile". Furthermore, by examining the limiting behaviour, we also find that for large N, no significant deviation arises in our system. If no limit exists, then there is also no clear macroscopic description of the system.To make this more rigorous, we first have to define what it means to have a given density profile. As an observable of the macroscopic behaviour of the interacting particle system, we consider the empirical density field, indicated for all N by μ^N and defined as follows.

$$\mu^N = \frac{1}{N} \sum_{x \in \mathbb{Z}} \eta_x \delta_{\frac{x}{N}} \tag{33}$$

Definition 3.2. Let $\phi \in \mathcal{S}(\mathbb{R})$. A sequence of configurations η^N is said to correspond to the density profile ρ if

$$\lim_{N \to \infty} < \mu^N, \phi >= \int_{\mathbb{R}} \phi(x)\rho(x)dx \tag{34}$$

We say that a sequence of probability distributions ν^N corresponds to the density profile ρ if

$$\mathbb{P}_{\nu^N}\left(| < \mu^N, \phi > - \int \phi(x)\rho(x)dx| \geq \epsilon \right) \to 0 \text{ as } N \to \infty \tag{35}$$

Remark 3.3. The Schwartz space, denoted by $\mathcal{S}(\mathbb{R})$, is the space of all rapidly decreasing smooth functions on $\mathbb{R}$. A function $f : \mathbb{R} \to \mathbb{R}$ belongs to $\mathcal{S}(\mathbb{R})$ if:

1. $f \in \mathcal{C}^\infty$ (infinitely differentiable)
2. For all $\alpha, \beta \in \mathbb{R}$, the function

$$x \to x^\alpha D^\beta f(x) \tag{36}$$

is bounded on $\mathbb{R}$, i.e.

$$\sup_{x\in\mathbb{R}}|x^\alpha D^\beta f(x)| < \infty \tag{37}$$

This means that both the function and all its derivatives decay faster than any polynomial grows.

Remark 3.4. Definition 3.2 holds for example for $\nu^N = \otimes_x Ber(\rho(\frac{x}{N}))$ since

$$\begin{aligned} \mathbb{E}\left(\frac{1}{N}\sum_x \eta_x\, \phi(\tfrac{x}{N})\right) &= \frac{1}{N}\sum_x \rho(\frac{x}{N})\, \phi(\frac{x}{N}) \\ &\to 0 \text{ as } N \to \infty \end{aligned} \tag{38}$$

where we used the linearity of the expectation value and the expectation value of the Bernoulli distribution, and

$$\begin{aligned} \mathrm{Var}\left(\frac{1}{N}\sum_x \eta_x\, \phi(\tfrac{x}{N})\right) &= \frac{1}{N^2}\sum_x \rho(\tfrac{x}{N})(1-\rho(\tfrac{x}{N})\phi^2(\tfrac{x}{N}) \\ &= \frac{1}{N}\int \phi^2(x)\rho(x)(1-\rho(x))dx + o(1/N) \\ &\to 0 \text{ as } N \to \infty \end{aligned} \tag{39}$$

here we used that the variation of a Bernoulli distribution with parameter $\rho(\frac{x}{N})$ is equal to $\rho(\frac{x}{N})(1-\rho\frac{x}{N})$. However, ν^N can be any product distribution, i.e. $\nu^N = \otimes_x \nu_x^N$, as long as $\nu_x^N(\eta_x) = \rho(\frac{x}{N})$ and $\mathrm{Var}(\eta_x)$ is finite.

Theorem 3.5 (Expectation value of the hydrodynamic limit of the SEP in a homogeneous environment)**.** *Let $\mu^N(t)$ be the empirical density profile and let $\eta \xrightarrow{d} \nu^N = \otimes_x Ber(\rho(\frac{x}{N}))$ at time $t = 0$ and let $\phi \in \mathcal{S}(\mathbb{R})$ be a function, then*

$$\lim_{N\to\infty} \mathbb{E}\langle \mu^N(t), \phi\rangle \to \int \rho_t(x)\phi(x)dx. \tag{40}$$

where $\rho_t(x)$ is the solution to the following partial differential equation:

$$\frac{\partial\rho}{\partial t} = \frac{\partial^2\rho}{\partial x^2} \tag{41}$$

Proof. The proof of the theorem will be split into two steps. The first step is about the reduction to a single-particle problem, using the duality relation. In the second step, we prove the convergence of the scaled random walk to Brownian motion through the convergence of the generator.

Step 1: Reduction to a single-particle problem

$$\begin{aligned}\mathbb{E}\langle \mu^N(t), \phi\rangle &= \mathbb{E}\left[\frac{1}{N}\sum_x \eta_x(tN^2)\phi\left(\frac{x}{N}\right)\right] \\ &= \frac{1}{N}\sum_x \int \mathbb{E}_\eta\left(\eta_x(tN^2)\right)\phi\left(\frac{x}{N}\right)\, d\nu^N(\eta) \end{aligned} \tag{42}$$

where in the last equality we used Fubini's integral theorem and linearity of the expectation value. Next we integrate over the measure ν^N and use the duality relation we derived earlier to obtain the following equality

$$\begin{aligned}&\frac{1}{N}\sum_x \int \mathbb{E}_\eta\left(\eta_x(tN^2)\right)\phi\left(\frac{x}{N}\right)\, d\mu^N(\eta) = \\ &\frac{1}{N}\sum_x \mathbb{E}_x^{RW}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right)\end{aligned} \tag{43}$$

Since our system is translation invariant we can shift the random walk:

$$\begin{aligned}&\frac{1}{N}\sum_x \mathbb{E}_x^{RW}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right) = \\ &\frac{1}{N}\sum_x \mathbb{E}_0^{RW}\left(\rho\left(\frac{X(tN^2)}{N}+\frac{x}{N}\right)\right)\phi\left(\frac{x}{N}\right)\end{aligned} \tag{44}$$

Step 2: Convergence of scaled random walk to Brownian motion
We want to show that

$$\frac{1}{N}\sum_x \mathbb{E}_0^{RW}\left(\rho\left(\frac{X(tN^2)}{N}+\frac{x}{N}\right)\right)\phi\left(\frac{x}{N}\right) \to \tag{45}$$

$$\int \mathbb{E}_0^{BM}\left(\rho(B(2t)+x)\right)\phi(x) \quad \text{as } N\to\infty \tag{46}$$

In order to prove this last convergence step we show that the Markov generator of the scaled random walk converges to the Markov generator of the corresponding Brownian motion. If we can show this generator convergence for a sufficient class of functions f, we can conclude the theorem. The Markov generator of the scaled random walk is given by

$$\mathcal{L}_N^{RW} f(x) = N^2\left(f(x+\tfrac{1}{N}) - 2f(x) + f(x-\tfrac{1}{N})\right) \tag{47}$$

Now if we consider a sequence of points $x_N \in \mathbb{Z}/N = \{\frac{x}{N}, x \in \mathbb{Z}\}$ such that $x_N \to y \in \mathbb{R}$, then we have that

$$\mathcal{L}_N^{RW} f(x_N) \to \frac{\partial^2 f(y)}{\partial x^2} \tag{48}$$

which is the generator of the Brownian motion process $B(2t)$. The convergence of equation 48 can be proven using a Taylor expansion. Using Theorem 2.10, we conclude that $\rho_t(x) = \mathbb{E}_0^{BM} \rho(B(2t) + x)$ is indeed the solution of 41. □

Remark 3.6.

$$\{\mu^N(t), 0 \leq t \leq T\} \to \{\rho_t(x), 0 \leq t \leq T\} \tag{49}$$

converges in path space in the sense of weak convergence. The thing to be added is the tightness of the trajectories which follow from studying the quadric variation of the martingale

$$M_t = < \mu^N(t), \phi > - < \mu^N(0) - \phi > - \int_0^t < \mu^N(s), \Delta^N \phi > ds \tag{50}$$

which can be shown to be of order $\frac{1}{N}$.

4 Symmetric exclusion process on a random environment

4.1 Model

We can extend the one-dimensional SEP in the homogeneous environment $\mathbb{Z}$ to a symmetric exclusion process in a random environment, abbreviated by SEP($\boldsymbol{\alpha}$), by assigning a maximal occupancy $\alpha_x \in \mathbb{N}$ to each site $x \in \mathbb{Z}$. In what follows, we refer to the random environment as the collection $\boldsymbol{\alpha} = \{\alpha_x, x \in \mathbb{Z}\}$. We assume that all instances of the random environment are iid and satisfy the following upper and lower bounds.

$$1 \leq \alpha_x \leq \mathcal{M}, \qquad x \in \mathbb{Z} \tag{51}$$

In this case, we define the configuration space $\chi^{\boldsymbol{\alpha}}$ as

$$\chi^{\boldsymbol{\alpha}} := \prod_{x \in \mathbb{Z}} \{0, ..., \alpha_x\} \tag{52}$$

Here the superscript emphasizes the dependence of the configuration space on the realization of the environment. We highlight that for the choice of $\alpha_x = 1$ for any $x \in \mathbb{Z}$, we recover the SEP on a homogeneous environment from chapter 3. Given an instance $\boldsymbol{\alpha}$ of the random environment, the Markov generator of the SEP($\boldsymbol{\alpha}$) is as follows:

$$\begin{aligned} \mathcal{L}f(\eta) = \sum_{x \in \mathbb{Z}} \Big[& \eta_x(\alpha_{x+1} - \eta_{x+1}) \left(f(\eta^{x,x+1}) - f(\eta) \right) \\ & + \eta_{x+1}(\alpha_x - \eta_x) \left(f(\eta^{x+1,x}) - f(\eta) \right) \Big] \end{aligned} \tag{53}$$

The transition rates between neighbouring sites are now modulated by the random environment. This extension is of great physical importance since it allows us to model disorder and impurities in a system. For example, structures such as semiconductors and metals are often affected by microscopic irregularities (e.g., atomic defects, impurities, or structural faults). These irregularities lead to spatially varying diffusion. Using the SEP($\boldsymbol{\alpha}$) we can effectively model such irregularities.

4.2 Self-duality of the SEP($\boldsymbol{\alpha}$)

The SEP($\boldsymbol{\alpha}$) is still a self-dual Markov process, which is stated in Lemma 4.1.

Lemma 4.1 (Duality relation of the *SEP*($\boldsymbol{\alpha}$))**.** *The SEP*($\boldsymbol{\alpha}$) *is a self-dual Markov process with self-duality function* $D : \chi_f \times \chi \to \mathbb{R}$ *given by*

$$D^{\boldsymbol{\alpha}}(\xi, \eta) := \prod_{x \in \mathbb{Z}} \frac{\binom{\eta_x}{\xi_x}}{\binom{\alpha_x}{\xi_x}} \cdot \mathbf{1}_{\{\xi_x \leq \eta_x\}} \tag{54}$$

Proof. For the proof we refer to [5]. □

Again, we are interested in the case where the dual system consists of only one particle (i.e. $\xi = \delta_x$). If there is only one particle in the system no interaction takes place and we are left with a single random walk on the random environment $\boldsymbol{\alpha}$, abbreviated by RW($\boldsymbol{\alpha}$). RW($\boldsymbol{\alpha}$) is the Markov process $\{X_t^{\boldsymbol{\alpha}}, t \geq 0\}$ on $\mathbb{Z}$ with the generator given by

$$\mathcal{L}^{RW(\boldsymbol{\alpha})} f(x) = \sum_{x \in \mathbb{Z}} \alpha_{x+1} \left(f(x+1) - f(x)\right) + \alpha_{x-1}(f(x-1) - f(x)) \tag{55}$$

where $f : \mathbb{Z} \to \mathbb{R}$ is again a bounded function. We can conclude the following semigroup duality relation:

$$\mathbb{E}_{\eta}^{SEP(\boldsymbol{\alpha})} \left(\eta_x(t)\right) = \mathbb{E}_x^{RW(\boldsymbol{\alpha})} \left(\eta_{x(t)}(0)\right) \tag{56}$$

4.3 Results from the Random Conductance Model

In order to prove the hydrodynamic limit of the SEP, we used generator convergence to conclude the convergence to Brownian motion. However, this does not work in a random environment. So, to prove the hydrodynamic limit of SEP($\boldsymbol{\alpha}$), we use an important result derived from studying the random conductance model (RCM).

The RCM is obtained by assigning a random conductance $\omega_{x,x+1}$ to each edge of $\mathbb{Z}$. We then say that the jump rate of a particle from $x \in \mathbb{Z}$ to a nearest neighbouring site y is given by $\omega_{x,y}$. Furthermore, we assume that all the conductances are iid, stationary and ergodic. The Markov generator of a random walk in the RCM is given by

$$\mathcal{L}f(x) = \omega_{x,x+1}(f(x+1) - f(x)) + \omega_{x,x-1}(f(x-1) - f(x)) \tag{57}$$

The following lemma states that a properly scaled version of this random walk converges to Brownian motion.

Lemma 4.2 (Convergence of random walk in RCM)**.** *Let $\{X(t), t \geq 0\}$ be the Markov process generated by the generator defined in 57. Then the rescaled random walk$\{\frac{X(tN^2)}{N}, t \geq 0\}$ converges to the Brownian motion process $B(Dt)$, where D is the diffusion coefficient.*

To proof lemma 4.2 we use a result from [10], which is stated here as Proposition 4.1.

Proposition 4.1. Let $\{M_t, t \geq 0\}$ be a martingale with stationary and ergodic increments. Then $\frac{M_{tN^2}}{N} \to B(\mathcal{D}t)$, where $\mathcal{D}$ is the diffusion coefficient given by

$$\mathcal{D} = \lim_{t \to \infty} \frac{\mathbb{E}(M_t^2)}{t} \tag{58}$$

Proof of lemma 4.2. We consider the martingale

$$\psi(\omega, x) = \begin{cases} \sum_{i=1}^{x} \frac{1}{\omega_{i,i+1}} & \text{if } x \geq 1 \\ 0 & \text{if } x = 0 \\ \sum_{i=x}^{-1} \frac{1}{\omega_{i,i+1}} & \text{if } x \leq -1 \end{cases} \tag{59}$$

Then for large N it holds that

$$< \frac{1}{\omega_{0,1}} > \frac{X(tN^2)}{N} \approx \frac{1}{N}\psi(\omega, X(tN^2)) \tag{60}$$

and using proposition 4.1 this converges to Brownian motion with diffusion coefficient D. □

4.4 Hydrodynamic limit of the SEP(α)

We are now in a position to prove the hydrodynamic limit of the SEP($\boldsymbol{\alpha}$).

Theorem 4.3 (Hydrodynamic limit of the SEP($\boldsymbol{\alpha}$) on a random environment)**.** *Let $\mu^N(t)$ be the empirical density field and let $\eta \xrightarrow{d} \nu^N = \otimes_x Ber(\rho(\frac{x}{N}))$ at time $t = 0$ and let ϕ be a function, then*

$$\lim_{N\to\infty} \mathbb{E}\langle \mu^N(t), \phi\rangle \to \int \rho_t(x)\phi(x)dx \tag{61}$$

where $\rho_t(x)$ is the solution to the following partial differential equation:

$$\frac{\partial \rho}{\partial t} = \frac{D}{2}\frac{\partial^2 \rho}{\partial x^2} \tag{62}$$

with D the diffusion constant.

Proof. The first steps of the proof are analogous to the first steps of the proof of theorem 3.5.

$$\begin{aligned} \mathbb{E}\left[\frac{1}{N}\sum_x \eta_x(tN^2)\phi\left(\frac{x}{N}\right)\right] &= \frac{1}{N}\sum_x \mathbb{E}\left(\eta_x(tN^2)\right)\phi\left(\frac{x}{N}\right) \\ &= \frac{1}{N}\sum_x \int \mathbb{E}_\eta\left(\eta_x(tN^2)\right)\phi\left(\frac{x}{N}\right) d\nu^N(\eta) \\ &= \frac{1}{N}\sum_x \mathbb{E}_x^{RW(\boldsymbol{\alpha})}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right) \end{aligned} \tag{63}$$

In order to conclude the convergence to Brownian motion, we point out that the generator of the RW on a random environment (eq. 55) is just a scalar multiple

of the generator of the RW in the RCM (eq. 57). Thus, using lemma 4.2, we can conclude the convergence to Brownian motion with diffusion coefficient D. Thus,

$$\begin{aligned}\frac{1}{N}\sum_x \mathbb{E}_x^{RW(\boldsymbol{\alpha})}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right) &= \frac{1}{N}\sum_x \left[\mathbb{E}_0^{BM}\left(\rho(B(Dt)+\tfrac{x}{N})\right)\phi(\tfrac{x}{N})\right] + o(1) \\ &\to \int \mathbb{E}_0^{BM}(\rho(B(Dt)+x))\phi(x)dx \qquad (64)\end{aligned}$$

Using Theorem 2.10, we see that $\rho_t(x) = \mathbb{E}_0^{BM}\rho(B(Dt)+x)$ is indeed the solution to 62. □

Remark 4.4. Notice that the diffusion coefficient is effectively averaged out through the homogenization process. We obtain a diffusion constant that depends on the the distribution of $\boldsymbol{\alpha}$. In the hydrodymamic limit, this diffusion coefficient becomes constant because $\boldsymbol{\alpha}$ is i.i.d..Functions that depend only weakly on a single random variable tend to become constant in the limit .

5 Symmetric exclusion process with reservoirs

5.1 The Model

Having examined the dynamics of the SEP process on both a homogeneous and a random environment, we now turn to the influence of reservoirs at the boundary of our system, where particles can enter and leave the system. Let $N \in \mathbb{N}$. We consider a linear chain by $I_N = \{1, 2, ...N-1\}$ put in contact, at its left and right boundaries, with two particle reservoirs, say reservoir L coupled to site 1 and reservoir R couples to site $N-1$. Particles can thus leave or enter the system only through the boundary sites 1 and $N-1$. We will call the set I_N the 'bulk' of our system and consider the symmetric exclusion process on this bulk, abbreviated by $\text{SEP}^{L,R}$. Note that the maximum occupancy in the bulk is still 1. We define the configuration space as follows

$$\chi^{L,R} := \prod_{x \in I_N} \{0, 1\} \tag{65}$$

We split the Markov generator of $\text{SEP}^{L,R}$ into three parts.

$$\mathcal{L} = \mathcal{L}_L + \mathcal{L}_R + \mathcal{L}_{\text{bulk}} \tag{66}$$

Where $\mathcal{L}_{bulk}$ describes the symmetric exclusion process in I_N, while $\mathcal{L}_L$ and $\mathcal{L}_R$ describe the actions of the reservoirs L and R on the boundaries, where particles can leave and enter the system.

$$\begin{aligned}\mathcal{L}_{\text{bulk}} f(\eta) = \sum_{x=1}^{N-2} \big[&\eta_x(1-\eta_{x+1})(f(\eta^{x,x+1}) - f(\eta)) \\ &+\eta_{x+1}(1-\eta_x)(f(\eta^{x+1,x}) - f(\eta))\end{aligned} \tag{67}$$

$$\mathcal{L}_L f(\eta) = \gamma_1(1-\eta_1)(f(\eta+\delta_1) - f(\eta)) + \delta_1\eta_1(f(\eta-\delta_1) - f(\eta)) \tag{68}$$

$$\mathcal{L}_R f(\eta) = \gamma_R(1-\eta_{N-1})(f(\eta+\delta_{N-1}) - f(\eta)) + \delta_R\eta_{N-1}(f(\eta-\delta_{N-1}) - f(\eta)) \tag{69}$$

The positive numbers γ_L, δ_L, γ_R and δ_R describe the rate at which particles can enter and leave the system. The reservoir generators act in such a ways as to "impose" to the boundary sites two fixed particle densities, ρ_L at the left and ρ_R at the right, with

$$\rho_L = \frac{\gamma_L}{\gamma_L + \delta_L} \quad \rho_R = \frac{\gamma_R}{\gamma_R + \delta_R} \tag{70}$$

This modified model captures the dynamics of open systems,i.e. systems that exchange particles with their environment. By setting different particle densities at the left and right boundary, a non-equilibrium stationary state (NESS) emerges. This leads to a effective current through the systems. In this way, we can model physical systems where gradients (e.g., of chemical potential or temperature) drive transport, such as in electrical conductors.

5.2 Duality relation of the SEP^{L,R}

Since particles can leave and enter the system, the $SEP^{L,R}$ is no longer a self-dual process. But, the dual process is a process in which the reservoirs are replaced with absorbing sites. This duality relation is formalized in Lemma 5.1.

Lemma 5.1 (Duality relation of the SEP^{L,R})**.** *$SEP^{L,R}$ has a dual process with generator:*

$$\begin{aligned}\mathcal{L}_{dual}f(\xi) = \sum_{x=1}^{N-2}(\xi_x(1-\xi_{x+1})(f(\xi^{x,x+1})-f(\xi)) \\ +\xi_{x+1}(1-\xi_x)(f(\xi^{x,x+1})-f(\xi))) \\ +(\gamma_L+\delta_L)(f(\xi-\delta_1)-f(\xi))+(\gamma_R+\delta_R)(f(\xi-\delta_{N-1})-f(\xi))\end{aligned} \tag{71}$$

and duality function

$$D(\xi,\eta) = \rho_L^{\xi_0}\rho_R^{\xi_N}\prod_{x=1}^{N-1}\frac{\binom{\eta_x}{\xi_x}}{\binom{1}{\xi_x}}\mathbf{1}_{\xi_\mathbf{x}\leq\eta_\mathbf{x}} \tag{72}$$

since $\eta_x, \xi_x \in \{0,1\}$ for all $x \in I_N$ this reduces to

$$D(\xi,\eta) = D(\xi,\eta) = \rho_L^{\xi_0}\rho_R^{\xi_N}\prod_{x=1}^{N-1}\eta_x \tag{73}$$

Proof. See Appendix □

When the dual configuration consists of a single particle, i.e $\xi = \delta_x$ for some $x \in I_N$, the generator of the dual process reduces to the generator of a random walk with absorbing sites at 0 and N, abbreviated by $RW(0,N)$, and given by

$$\mathcal{L}_{\text{dual}}^{RW(0,N)}f(x) = \begin{cases} f(x+1)-f(x)+f(x-1)-f(x) & \text{if } x\in\{1,2,\ldots,N-1\} \\ 0 & \text{if } x=0 \\ 0 & \text{if } x=N \end{cases} \tag{74}$$

In this case we can conclude the following semigroup duality relation

$$\mathbb{E}_\eta\left(\eta_x(t)\right) = \mathbb{E}_x^{\text{RW(0,N)}}\left(\eta_{x(t)}(0)\right) \tag{75}$$

5.3 Hydrodynamic Limit of SEP^{L,R}

In the case of $SEP^{L,R}$ we are interested in the macroscopic behaviour of the bulk. Thus we define the empirical density field $\mu^N(t)$ as

$$\mu^N(t) = \frac{1}{N}\sum_{x=1}^{N-1}\eta_x(tN^2)\delta_{x/N} \tag{76}$$

Theorem 5.2 (Hydrodynamic limit of $SEP^{L,R}$)**.** *Let $\mu^N(t)$ be the empirical measure defined in 76 and let $\eta \xrightarrow{d} \mu^N = \otimes_{x\in I_N} Ber(\rho(\frac{x}{N}))$ at time $t = 0$. and let ϕ be a function, then*

$$\lim_{N\to\infty} \mathbb{E}\langle \mu^N(t), \phi\rangle \to \int \rho_t(x)\phi(x)dx \tag{77}$$

where $\rho_t(x)$ is the solution to the following partial differential equation with Dirichlet boundary conditions:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{\partial^2 \rho}{\partial x^2} \\ \rho_t(0) &= \rho_L \\ \rho_t(1) &= \rho_R \end{aligned} \tag{78}$$

Proof. The proof will be split into two main steps. The first step is about the reduction to a single particle problem using the duality relation. In the second part, we prove the convergence of the scaled random walk to the absorbed Brownian motion process.

Step 1: Reduction to a single-particle problem
In order to reduce to problem to a single particle problem we take similar steps as in Theorem 3.5

$$\begin{aligned} \mathbb{E}\langle \mu^N(t), \phi\rangle &= \mathbb{E}\left[\frac{1}{N}\sum_{x=1}^{N-1} \eta_x(tN^2)\phi\left(\frac{x}{N}\right)\right] \\ &= \frac{1}{N}\sum_{x=1}^{N-1}\int \mathbb{E}_\eta\left(\eta_x(tN^2)\right)\phi\left(\frac{x}{N}\right) d\nu^N(\eta) \\ &= \frac{1}{N}\sum_{x} \mathbb{E}_x^{RW(0,N)}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right) \end{aligned} \tag{79}$$

Step 2: Convergence of the scaled random walk to Brownian motion
In order to prove the convergence to Brownian motion, we show that the generator of the properly scaled RW(O,N), converges to the corresponding generator of the absorbed Brownian motion process. If we can show this generator convergence for a sufficient class of functions we can conclude process convergence, and thus prove the theorem. The Markov generator of the properly scaled RW(0,N) is given by

$$\mathcal{L}_N^{RW(0,1)} f(x) = \begin{cases} N^2\left[f\left(x+\frac{1}{N}\right) - f(x) + f\left(x-\frac{1}{N}\right) - f(x)\right] & \text{if } x \in \left\{\frac{1}{N}, \ldots, \frac{N-1}{N}\right\} \\ 0 & \text{if } x = 0 \\ 0 & \text{if } x = 1 \end{cases} \tag{80}$$

If we let x_N be a sequence in $\{0, \frac{1}{N}, \frac{2}{N}, ...\frac{N-1}{N}, 1\}$ such that $x_N \to y \in [0,1]$ and let $f \in \mathcal{C}^2$ such that $f''(0) = f''(1) = 0$, then

$$\mathcal{L}_N f(x_N) \to \mathcal{L}f(x) = \begin{cases} f''(x) & \text{if } x \in (0,1) \\ 0 & \text{if } x = 0 \\ 0 & \text{if } x = 1 \end{cases} \tag{81}$$

Which is the generator of the Brownian motion process $B(2t)$ with absorbing sites at 0 and 1. Again, the convergence of 81 can be proven using a Taylor expansion. Using Theorem 2.11 and the fact that the reservoirs ensure a particle density of ρ_L and ρ_R, we conclude that $\rho_t(x) = \mathbb{E}_x^{BM(0,1)}\rho(B(2t) + x)$ is indeed the solution of 92. □

6 Symmetric exclusion process on a random environment with reservoirs

6.1 The model

We can extend the SEP^{L,R} by a assigning a maximum occupancy $\alpha_x \in \mathbb{N}$ to each site $x \in I_N = \{1, 2, ...N-1\}$, abbreviated by $SEP^{L,R}(\boldsymbol{\alpha})$, and thus combining the models of chapters 4 and 5. In what follows, we refer to the random environment as the collection $\boldsymbol{\alpha} = \{\alpha_x, x \in I_N\}$ for which we assume ergodicity and uniform ellipticity. We define the configuration space as follows.

$$\chi^{L,R}(\boldsymbol{\alpha}) := \prod_{x \in I_N} \{0, 1, ...\alpha_x\} \tag{82}$$

We split the generator of SEP$^{L,R}(\boldsymbol{\alpha})$ into three different parts.

$$\mathcal{L}^{\boldsymbol{\alpha}} = \mathcal{L}_L^{\boldsymbol{\alpha}} + \mathcal{L}_R^{\boldsymbol{\alpha}} + \mathcal{L}_{bulk}^{\boldsymbol{\alpha}} \tag{83}$$

Where $\mathcal{L}_{bulk}^{\boldsymbol{\alpha}}$ describes the symmetric exclusion process in random environment in I_N, while $\mathcal{L}_L^{\boldsymbol{\alpha}}$ and $\mathcal{L}_R^{\boldsymbol{\alpha}}$ describe the actions of the reservoirs.

$$\begin{aligned}\mathcal{L}_{\text{bulk}}^{\boldsymbol{\alpha}} f(\eta) = \sum_{x=1}^{N-2} \Big[&\eta_x(\alpha_{x+1} - \eta_{x+1}) \left(f(\eta^{x,x+1}) - f(\eta) \right) \\ &+ \eta_{x+1}(\alpha_x - \eta_x) \left(f(\eta^{x+1,x}) - f(\eta) \right) \Big]\end{aligned} \tag{84}$$

$$\mathcal{L}_L^{\boldsymbol{\alpha}} f(\eta) = \gamma_1(\alpha_1 - \eta_1)(f(\eta + \delta_1) - f(\eta)) + \delta_1 \eta_1 (f(\eta - \delta_1) - f(\eta)) \tag{85}$$

$$\mathcal{L}_R^{\boldsymbol{\alpha}} f(\eta) = \gamma_R(\alpha_{N-1} - \eta_{N-1})(f(\eta + \delta_{N-1}) - f(\eta)) + \delta_R \eta_{N-1}(f(\eta - \delta_{N-1}) - f(\eta)) \tag{86}$$

The positive numbers γ_L, δ_L, γ_R and δ_R have the same meaning as in the SEP^{L,R}. The presence of the random environment and reservoirs at the boundaries leads to a net current that must traverse regions of varying conductance, akin to charge or mass transport in inhomogeneous environments of irregular conductors.

6.2 Duality relation of the SEP$^{L,R}(\boldsymbol{\alpha})$

SEP$^{L,R}(\boldsymbol{\alpha})$ still has a dual Markov process where the reservoirs are replaced with absorbing sites. This duality relation is formalized in Lemma 6.1

Lemma 6.1 (Duality relation of $SEP^{L,R}(\boldsymbol{\alpha})$)**.** *$SEP^{L,R}(\boldsymbol{\alpha})$ has a dual process with generator:*

$$\begin{aligned}\mathcal{L}_{dual}f(\xi) = \sum_{i=1}^{N-2} \Big(&\xi_i(\alpha_{i+1}-\xi_{i+1})\left(f(\xi^{i,i+1})-f(\xi)\right)\\ &+\xi_{i+1}(\alpha_i-\xi_i)\left(f(\xi^{i,i+1})-f(\xi)\right)\Big)\\ &+(\gamma_L+\delta_L)\left(f(\xi^{1,0})-f(\xi)\right)\\ &+(\gamma_R+\delta_R)\left(f(\xi^{N-1,N})-f(\xi)\right)\end{aligned} \tag{87}$$

and duality function

$$D(\xi,\eta) = \rho_L^{\xi_0}\rho_R^{\xi_N}\prod_{x=1}^{N-1}\frac{\binom{\eta_x}{\xi_x}}{\binom{\alpha_x}{\xi_x}}\mathbf{1}_{\{\xi_\mathbf{x}\leq\eta_\mathbf{x}\}} \tag{88}$$

Proof. See Appendix □

When the dual configuration consists of a single particle, i.e. $\xi = \delta_x$ for some $x \in I_N$, the generator of the dual process reduces to the generator of a random walk on a random environment with absorbing sites at 0 and N, abbreviated by $\mathrm{RW}(\boldsymbol{\alpha})^{(0,N)}$. The generator of the dual configuration is, in this case, given by

$$\mathcal{L}_{\text{dual}}^{RW^{(0,N)}(\boldsymbol{\alpha})}f(x) = \begin{cases}\alpha_{x+1}(f(x+1)-f(x)) + \alpha_{x-1}(f(x-1)-f(x)) & \text{if } x\in\{1,2,\ldots,N-1\}\\ 0 & \text{if } x=0\\ 0 & \text{if } x=N\end{cases} \tag{89}$$

In this case we can conclude the following semigroup duality relation

$$\mathbb{E}_\eta\left(\eta_x(t)\right) = \mathbb{E}_x^{RW^{(0,N)}(\boldsymbol{\alpha})}\left(\eta_{x(t)}(0)\right) \tag{90}$$

6.3 Hydrodynamic limit of the $\mathrm{SEP}^{L,R}(\boldsymbol{\alpha})$

Since we are again interested in the macroscopic behaviour of the bulk I_N, we define the empirical density field $\mu^N(t)$ as in eq. 76.

Theorem 6.2 (Expectation value of the hydrodynamic limit of $\mathrm{SEP}^{L,R}(\boldsymbol{\alpha})$)**.** *Let $\mu^N(t)$ be the empirical measure density field and let $\eta \xrightarrow{d} \nu^N = \otimes_{X\in I_N} Ber((\rho(\frac{x}{N}))$ at time $t=0$, and let ϕ be a function, then*

$$\lim_{N\to\infty}\mathbb{E}\langle\mu^N(t),\phi\rangle \to \int \rho_t(x)\phi(x)dx \tag{91}$$

where $\rho_t(x)$ is the solution to the following partial differential equation with Dirichlet boundary conditions:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{D}{2}\frac{\partial^2 \rho}{\partial x^2} \\ \rho_t(0) &= \rho_L \\ \rho_t(1) &= \rho_R \end{aligned} \tag{92}$$

where D is the diffusion coefficient.

Proof. The first steps of the proof are similar to those of the proof of Theorem 3.5

$$\begin{aligned} \mathbb{E}\langle \mu^N(t), \phi \rangle = \mathbb{E}\left[\frac{1}{N} \sum_{x=1}^{N-1} \eta_x(tN^2)\phi\left(\frac{x}{N}\right)\right] = \\ \frac{1}{N}\sum_{x=1}^{N-1} \int \mathbb{E}_\eta\left(\eta_x(tN^2)\right)\phi\left(\frac{x}{N}\right)\, d\nu^N(\eta) = \\ \frac{1}{N}\sum_x \mathbb{E}_x^{RW^{(0,N)}(\boldsymbol{\alpha})}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right) \end{aligned} \tag{93}$$

In order to conclude the convergence to Brownian motion, i.e.

$$\begin{aligned} \frac{1}{N}\sum_x \mathbb{E}_x^{RW^{(0,N)}(\boldsymbol{\alpha})}\left(\rho\left(\frac{X(tN^2)}{N}\right)\right)\phi\left(\frac{x}{N}\right) \rightarrow \\ \int \mathbb{E}_x^{BM(0,1)}\rho(B(Dt)+x)\phi(x)dx \end{aligned} \tag{94}$$

we follow the following reasoning. As long as the random walk on a random environment is not absorbed by the absorbing boundary sites, it will converge to the Brownian motion process with diffusion coefficient D according to Theorem 4.3. When the random walk is absorbed by one of the boundary sites, it will also converge to the Brownian motion process, since for both processes the particle will stay at the absorbed site indefinitely. □

7 Physical application

In his chapter we look at an example of an area of practical application of the results that were found in the previous chapters. This example concerns the migration of Li^+ ions through an electrolyte in a lithium battery. This could be modelled using the $\text{SEP}^{L,R}$ and $\text{SEP}^{L,R}(\boldsymbol{\alpha})$, for instance to assess the effect of the level of disorder of the anion structure of the electrolyte on the ion conductivity.

7.1 Basic principles of lithium batteries

A lithium battery consists of several individual cells that are connected to one another. Each cell contains three main parts: a positive cathode, a negative anode, and an electrolyte. A discharging lithium battery provides power through the movement of lithium ions. During discharging lithium ions diffuse from the anode to the cathode because their electrochemical potential is higher at the anode, ρ_R, than at the cathode ρ_L [11]. This difference leads to the ion diffusion through the electrolyte. Electrons flow, from the anode to the cathode via an external circuit providing a current. Inside a lithium battery, reduction-oxidation reactions take place. The reduction reaction occurs at the cathode. There, cobalt oxide combines with lithium ions to form lithium-cobalt oxide. The notation for the chemical reaction is:

$$\text{CoO}_2 + \text{Li}^+ + \text{e}^- \longrightarrow \text{LiCoO}_2 \tag{95}$$

The oxidation reaction takes place at the anode. There, the graphite intercalation compound LiC_6 forms graphite C_6 and lithium ions. The notation for this chemical reaction is as follows:

$$\text{LiC}_6 \longrightarrow \text{C}_6 + \text{Li}^+ + \text{e}^- \tag{96}$$

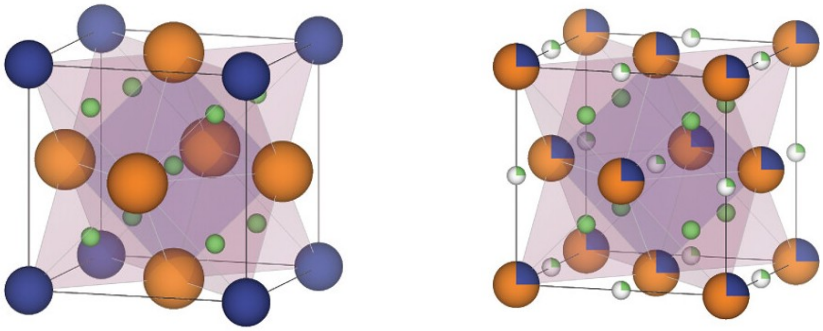
Since a battery can maintain the same electrochemical potential at the anode and cathode for a long time, the typical diffusion of Li^+ ions can be modelled using the $\text{SEP}^{L,R}$, assuming we have a fully homogeneous electrolyte.

7.2 Disorder in the electrolyte

However, the ionic conductivity of the electrolyte is a strong determinant of the performance of the lithium battery, i.e. the strength of the current that is generated. In particular, if we use $\text{Li}_9\text{S}_3\text{N}$ as our electrolyte, it turns out we can boost the ion conductivity by introducing disorder in the anion sublattices [7]. Then the assumption of a fully homogeneous electrolyte no longer applies. In this case, we can still model the diffusion of the Li^+ ions using the $\text{SEP}^{L,R}(\boldsymbol{\alpha})$. Thus, we can still assess the effect of the level of disorder on the performance of the battery in this case. Moreover, we could predict the macroscopic behaviour, see chapter 6, of the Li^+ ions and consequently use this knowledge to improve the design of the batteries and boost their performance. This type of knowledge

does not only bear academic relevance, but could also contribute to a better environment, considering the world's growing dependence on batteries.

Let us study in a bit more detail the effect of disorder on the ion conductivity in the electrolyte. We consider two polymorphs of Li_9S_3N: an anion-ordered phase and a disordered phase. The disorder arises from the random occupation of the anion sublattice by sulfur (S^{2-}) and nitrogen (N^{3-}) atoms. For all the points that make up the anion face-centered cubic lattice, the probability ration of being occupied by a S and N ion is 3:1, as can be seen in Figure 1. This is consistent with the overall structure of Li_9S_3N.



(a) (b)

Figure 1: Comparison between (a) ordered and (b) disordered electrolyte structures. Source [7].

This anion disorder gives rise to a diverse array of local environments of the diffusion Li^+ ions, and makes it dependent on the the specific configuration of the adjacent S and N atoms. This is because the lack of homogeneity in the microscopic environment directly affects the size of the bottlenecks that need to be passed by the Li^+ ions. Since ${N_3}^-$ is significantly smaller (ionic radius $\approx$ 1.46 Å) than ${S_2}^-$ ($\approx$ 1.84 Å), the inclusion of nitrogen increases the size of the bottlenecks and reduces repulsive interactions with other L^+ ions, thereby lowering the activation barrier for ion hops. irrespective of the local anion ordering, three general families of jumps are observed through the face-centered anion arrangement in Li_9S_3N. (i) tetrahedron-to-octahedron (tet-oct), (ii) octahedron-to-tetrahedron (oct-tet) and (iii) tetrahedron-to-tetrahedron (tet-tet) jumps. Figure 2 shows the activation barrier of individual jumps segregated by local environments. Because of its ordered S-N arrangement, ordered Li_9S_3N merely features 6 discrete jumps which are shown as discrete points in in Figure 2.

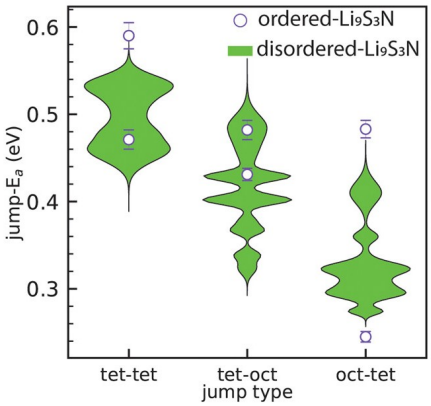


Figure 2: Comparison of the observable ion activation barriers for ion hops in ordered and disordered Li_9S_3N. The white points indicate the ion activation barrier of the six distinct jump types possible in ordered Li_9S_3N. In disordered Li_9S_3N, different jumps are observable and shown here as density plots. The horizontal scale represents the relative occurrence of jump types at that energy. Adapted from [7].

As a result, the diffusion of lithium ions through an electrolyte does not follow a uniform crystalline diffusion pattern. Instead, it resembles a random walk in a random environment, modulated by the direction of the electrochemical potential gradient, which determines the net flux direction. This matches the properties of the $\mathrm{SEP}^{L,R}(\boldsymbol{\alpha})$ and thus, we can use the $\mathrm{SEP}^{L,R}(\boldsymbol{\alpha})$ to model the migration of Li^+ ions through the disordered electrolyte. In this model, a higher random jump rate, due to the a higher maximum occupation, corresponds to the lower local activation energy due to atomic scale disorder. The parameters describing the reservoirs in the model, represent the electrochemical potential gradient. This way we can provide a rigorous framework for understanding how structural disorder affects ionic mobility. On the other hand, we can also use the model to predict which anion structure will lead to the best conductivity. Thus, it could inspire intensive interaction between physicist and mathematicians around a topic with potentially large societal relevance.

8 Conclusion

The main conclusions of this thesis project are as follows. First, that even for the fourth and most advanced model a proof of the hydrodynamic limit can be obtained. Furthermore, this project shows that to obtain this proof the use of duality is an effective approach. Finally, the results offer an opportunity to bridge the mathematical models and physical reality to improve the performance of lithium batteries.

At the same time, the results suggest opportunities for further research in several directions. Concerning mathematics, two issues are of particular relevance. First, the need to prove that the variance of the empirical density field goes to zero. In the project itself only the expectation value of the hydrodynamic limit has been determined. For a more complete result it is necessary to establish that the variance of this empirical density field stays within certain bounds.
Secondly, all results could be generalized to more dimensions. In the project itself only one-dimensional models were used. In order to more accurately model the migration of lithium ions through the electrolyte a three dimensional model is necessary. This is also related to opportunities for extensions in the physics domain. In particular, more detailed modelling of the ion migration in a lithium battery taking into account, still using the mathematical models outlined in this thesis but adding more details from physics about the behaviour of the ions.

9 Appendix

9.1 Proof of Lemma 3.1

Proof. in order to proof the proposition we must show that: $\mathcal{L}_\eta D(\cdot,\eta)(\xi) = \mathcal{L}_\xi D(\xi,\cdot)(\eta)$. Recall that

$$\mathcal{L}_\eta D(\xi,\eta) = \sum_{x\in\mathbb{Z}} \Big[\eta_x(1-\eta_{x+1})\left(D(\xi,\eta^{x,x+1}) - D(\xi,\eta)\right) + \eta_{x+1}(1-\eta_x)\left(D(\xi,\eta^{x+1,x}) - D(\xi,\eta)\right)\Big] \tag{97}$$

. When a particle jumps form site x to site $x+1$, the value of η_x decreases by 1 and the value of η_{x+1} will increase by 1. Thus we find the following expression for $D(\xi,\eta^{x,x+1})$

$$\begin{aligned} D(\xi,\eta^{x,x+1}) = &\prod_{y\neq x,x+1} \frac{\eta_y!}{(\eta_y-\xi_y)!}(1-\xi_y)!\mathbf{1}_{\{\xi_y\leq\eta_y\}} \\ &\frac{(\eta_x-1)!}{(\eta_x-1-\xi_x)!}(1-\xi_x)!\frac{(\eta_{x+1}+1)!}{(\eta_{x+1}+1-\xi_{x+1})!}(1-\xi_{x+1})! \\ &\mathbf{1}_{\{\xi_{x+1}\leq\eta_{x+1}+1\}}\mathbf{1}_{\{\xi_x\leq\eta_x-1\}} \end{aligned} \tag{98}$$

Thus,

$$\begin{aligned} D(\xi,\eta^{x,x+1}) - D(\xi,\eta) = D(\xi,\eta)\Bigg(&\frac{(\eta_x-\xi_x)(\eta_{x+1}+1)}{\eta_x(\eta_{x+1}+1-\xi_{x+1})} \\ &\frac{\mathbf{1}_{\{\xi_x\leq\eta_x-1\}}\mathbf{1}_{\{\xi_{x+1}\leq\eta_{x+1}+1\}}}{\mathbf{1}_{\{\xi_x\leq\eta_x\}}\mathbf{1}_{\{\xi_{x+1}\leq\eta_{x+1}\}}} - 1\Bigg) \end{aligned} \tag{99}$$

where we use that in the fraction $\frac{D(\xi,\eta^{x,x+1}}{D(\xi,\eta)}$ all terms cancel, expect for the sites x and $x+1$.We can calculate $D(\xi^{x,x+1},\eta)$, in the same way. Since $\xi_x,\eta_x\in\{0,1\}$, the only non zero contributions occur when $\xi_x=1,\xi_{x+1}=0$. In this case

$$D(\xi,\eta^{x,x+1}) = \begin{cases} D(\xi^{x,x+1},\eta) & \text{if } \eta_x=1,\ \eta_{x+1}=0 \\ 0 & \text{otherwise} \end{cases} \tag{100}$$

Thus for each allowed jump in η and corresponding allowed jump in ξ the increments in D match. And thus we find therefore,

$$\mathcal{L}_\eta D(\cdot,\eta)(\xi) = \mathcal{L}_\xi D(\xi,\cdot)(\eta) \tag{101}$$

which proves the self-duality relation. □

9.2 Proof of Lemma 5.1 and Lemma 6.1

We will proof the duality relation of Lemma 6.1, The duality relation of Lemma 5.1 follows by taking $\alpha_x = 1$ for all x

Proof of Lemma 6.1. From 4.1 we know that the $SEP(\boldsymbol{\alpha})$ is self dual with duality function

$$D^{\boldsymbol{\alpha}}(\xi,\eta) := \prod_{x\in\mathbb{Z}} \frac{\eta_x!}{(\eta_x-\xi_x)!}\frac{(\alpha_x-\xi_x)!}{\alpha_x!}\cdot \mathbf{1}_{\{\xi_x\leq\eta_x\}} \tag{102}$$

Thus, in order to prove the duality relation of $SEP^{L,R}(\boldsymbol{\alpha})$, it remains to verify that the actions of the operators $\mathcal{L}_L^{\boldsymbol{\alpha}}$ and $\mathcal{L}_R^{\boldsymbol{\alpha}}$ on the duality function $D(\xi,\eta)$ are the same as the actions of the dual operators at the boundaries. We will show this for the left boundary, the proof of the right boundary being analogous.

$$\begin{aligned}
\mathcal{L}_L^{\boldsymbol{\alpha}} D(\xi,\eta) &= \gamma_L(\alpha_1-\eta_1)\left[D(\eta+\delta_1,\xi)-D(\eta,\xi)\right] \\
&\quad + \delta_L\eta_1\left[D(\eta-\delta_1,\xi)-D(\eta,\xi)\right] \\
&= \gamma_L(\alpha_1-\eta_1)\left[\prod_{i=2}^{N-1}\frac{\eta_i!}{(\eta_i-\xi_i)!}(\alpha_i-\xi_i)!\frac{(\eta_1+1)!}{(\eta_1+1-\xi_1)!}(\alpha_1-\xi_1)! - D(\eta,\xi)\right] \\
&\quad + \delta_L\eta_1\left[\prod_{i=2}^{N-1}\frac{\eta_i!}{(\eta_i-\xi_i)!}(\alpha_i-\xi_i)!\frac{(\eta_1-1)!}{(\eta_1-1-\xi_1)!}(\alpha_1-\xi_1)! - D(\eta,\xi)\right] \\
&= \gamma_L(\alpha_1-\eta_1)D(\xi,\eta)\left[\frac{(\eta_1+1)!(\eta_1-\xi_1)!}{(\eta_1+1-\xi_1)!\eta_1!}-1\right] \\
&\quad + \delta_L\eta_1 D(\xi,\eta)\left[\frac{(\eta_1-1)!(\eta_1-\xi_1)!}{(\eta_1-1-\xi_1)!\eta_1!}-1\right] \\
&= \gamma_L(\alpha_1-\eta_1)D(\xi,\eta)\left[\frac{(\eta_1+1)-(\eta_1+1-\xi_1)}{(\eta_1+1-\xi_1)}\right] \\
&\quad + \delta_L\eta_1 D(\xi,\eta)\left[\frac{(\eta_1-\xi_1)-\eta_1}{\eta_1}\right] \\
&= \gamma_L(\alpha_1-\eta_1)D(\xi,\eta)\left[\frac{\xi_1}{(\eta_1+1-\xi_1)}\right] - \delta_L D(\xi,\eta)\xi_1 \\
&= D(\xi,\eta)\left[\frac{\gamma_L(\alpha_1-\eta_1)\xi_1}{(\eta_1+1-\xi_1)} - \delta_L\xi_1\right] \\
&= D(\xi,\eta)\frac{\xi_1}{(\eta_1+1-\xi_1)}\left[\gamma_L(\alpha_1-\eta_1)-\delta_L(\eta_1+1-\xi_1)\right] \\
&= D(\xi,\eta)\frac{\xi_1}{(\eta_1+1-\xi_1)}\left[\gamma_L(\alpha_1+1-\xi_1)-(\eta_1+1-\xi_1)\right] \\
&= \xi_1\left[\gamma_L\frac{(_1+1-xi_1)}{(\eta_1+1-\xi_1)}D(\xi,\eta)-D(\xi,\eta)\right] \\
&= \mathcal{L}_L^{\boldsymbol{\alpha},dual}D(\xi,\eta)
\end{aligned} \tag{103}$$

which concludes the proof.

□

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