Bose-Einstein condensate of annihilating particles

Modelled as a zero range process

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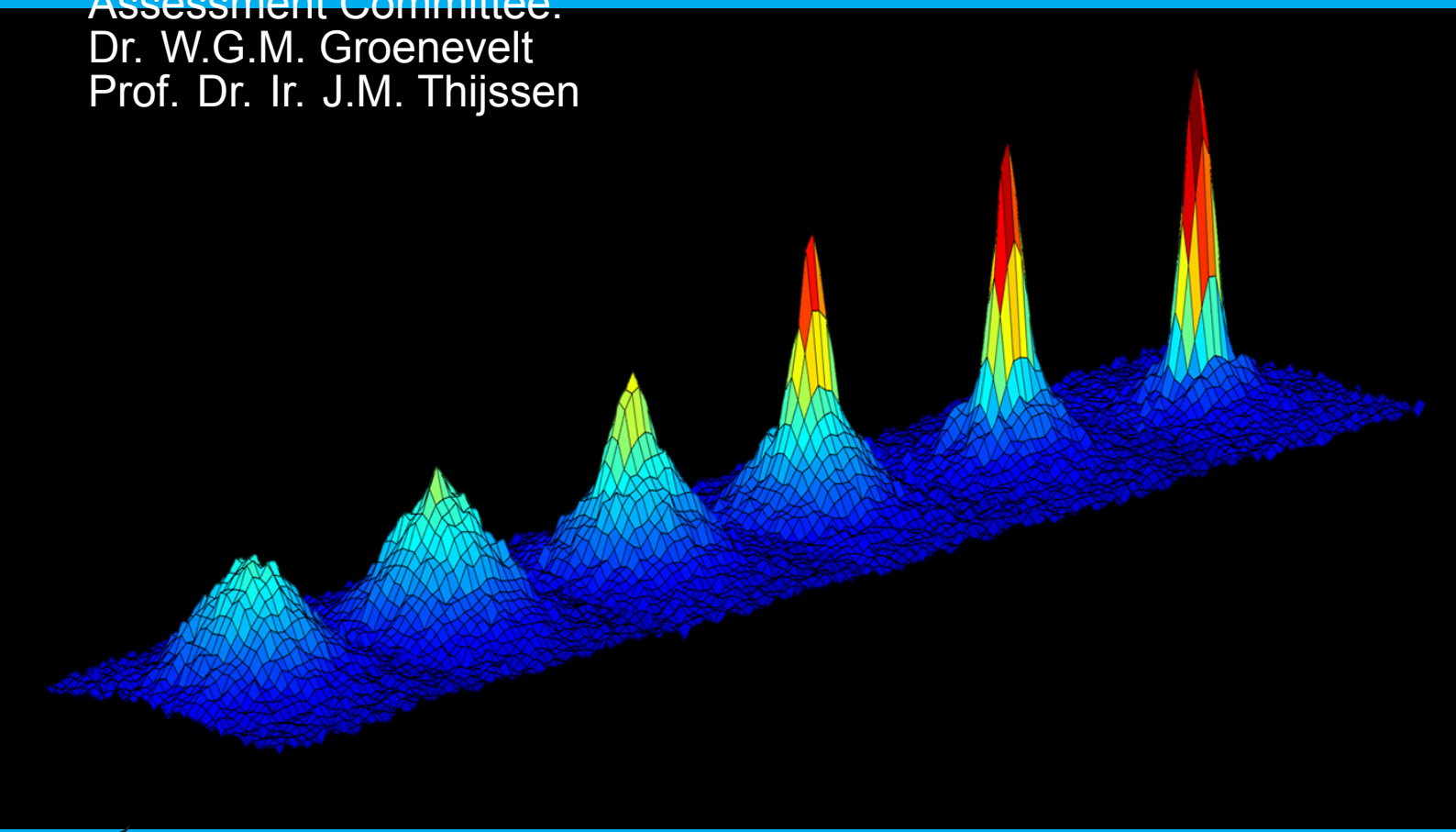

TU Delft

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by

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Preface

In the course Statistical Physics I got a basic understanding of the concept of Bose-Einstein condensate. This specific part I found interesting because it was not intuitive to me. Therefore I wanted to understand this better, and as I had to start my thesis I figured this is a great way to understand this concept better.

With this idea I approached Stephan Eijt as he was one of the tutors of the statistical physics course. He introduced the idea to study annihilating particles, or specifically positronium particles. As a Bose-Einstein condensate is the equilibrium position of a system we cannot do this with just the knowledge from equilibrium statistical physics. Therefore Stephan Eijt introduced Frank Redig from the math department of applied probability. He introduced me to the Zero-Range process.

After understanding the basics of the Zero range process that I documented with intensive help from Frank Redig. Now we started to explore what happens when an annihilation term is introduced to these kind of systems we constructed an easy single slow site zero range process. Frank Redig introduced us to Stefan Grosskinsky, who helped me in this part with the simulations of this exact same system, and together with Frank Redig discussed the proof that the equations we came up with are the limit of the large system.

After that I build a zero range process that behaves the same as a 3D harmonic oscillator with a finite amount amount of particles in equilibrium. This result can be interpreted with results from statistical physics, and therefore be of use for statistical physics.

K.Koot

Abstract

In this thesis the behaviour of a Bose Einstein condensate is explored that consists of bosons that annihilate. In order to do this a system where bose einstein condensation occurs is modeled as a Zero Range process which is a special case of a Markov process.

First we made a single slow site Zero range process with uniform rates and see how this would be influenced by annihilating particles. For this system it is shown that, in the large system limit, the number of particles in the slow site is given by a differential equation. A series of realization of different sizes of this system are done to support that the fraction of the particles in the ground state converges to the differential equation.

In order to relate this mathematical approach to physical Bose Einstein condensates it is established that the equilibrium distributions of multiple bosons in one system is the same as the detailed balance of a zero range process where the transition rates depend on the occupation of a site, with an indication function, that is equal to 0 when there are no particles at that site and some constant c if there is one or more particles at that site.

In statistical physics we need to take the energy of the state of the system into account. If the particles do not have interaction with each other this is the sum over all particles of the energy of the particle site. As a zero range model only has rates with one particle hop we can see that the difference in energy of the system is equal to the difference in energy of the sites of hop. In order to stay in detailed balance the rate for the specific hop must be $e^{-\beta\Delta E}$ times the opposite rate, where $\beta = \frac{1}{k_B T}$.

Now we can go from any system with a set of spin orbitals and energies of those spin orbitals and design a zero range model where the spin orbitals correspond to sites of the zero range model with rates between those sites, such that the systems detailed balance distribution is the same distribution as the equilibrium of the physical system. In this zero range model an annihilation term is introduced. This can be any function of occupation for the site, but in this report a simple relation that decreases when ΔE increases is used.

In order to see the effect on such systems the system is numerically approached for a 100 particles system in a 3 dimensional harmonic potential. This system is too complicated to get an differential equation that can be easily solved. Therefore it is approximated. This numerical approximation appears to have similar behaviour to the numerical approximation done in [3]. However the results are not identical.

The advantage of the model in this thesis is that an annihilation therm can be implemented. This approximation of a 3 dimensional harmonic oscillator with annihilating particles is done. If annihilation is slow enough, the exited sites form a different equilibrium compared to a Bose Einstein condensate of non annihilating particles. This happens as long as there is a condensate in the ground state.

Contents

1 Introduction

In 1924 Albert Einstein together with Satyendra Nath Bose came up with the Bose Einstein distribution and also theorized that when a boson gas becomes sufficiently dense and cold it would form a state of matter known as the Bose Einstein condensate.

A Bose Einstein condensate (BEC) is a state of matter only bosons can be in. It only occurs when they are very cold and dense. At that High density and low temperature if one would increase the density of that boson even further by adding particles all those particles would go to the 'lowest energy state'.

Positronium is a boson consisting of an electron and a positron (also known as an anti-electron). This means we have a particle that consists of matter and anti matter. As expected these particles are unstable and have an average lifespan of $1.42 * 10^{-7} s$ when the positron and electron have parallel spins also known as the triplet states (total spin $s = 1$). When the positron and electron have anti parallel spins it is in the singlet state ($s = 0$) and the average lifespan is $1.24 * 10^{-10} s$.

Bose Einstein condensates come from the theory that assuming all particles are in thermodynamic equilibrium. However when we have particles that disappear very fast it might not be reasonable to presume that the system goes to the same equilibrium, as we introduce an inherent change in the system.

Bose Einstein condensation occurs because the number of particles is presumed large, known as the thermodynamic limit. Because we cannot consider the quantum mechanical forces that act on every state we design we do not consider quantum mechanics that would contribute to any state change. Therefore we presume the only thing that changes the state is a given and only depends on the occupation of that site. This corresponds to the Zero Range process.

The goal of this report is to compute how a system that without annihilation forms a Bose Einstein condensate will behave when we introduce annihilation's that are of similar order as the time it takes for the 'normal' system to go to equilibrium, and then use that to make a prediction of what happens when a system where the rates of the system to go to equilibrium are of the same order as the time until the particles annihilate, like a BEC consisting of positronium might.

1.1. Positronium and spin

There has to date not been an experiment where positronium is made into a BEC. Therefore we will do a short exploration of some fundamentals of how such a state would be reached.

A way to make a Bose Einstein condensate of positronium is by isolating positronium particles in the

triplet state that all have the same spin 1. Spin 1 particle are magnetic dipoles. Therefore they can be trapped in a magnetic field in order to create a dense gas. This way we can use magnetism to create a harmonic oscillator for the positronium with that spin. Because we would need to make this as dense as possible it will probably be best to have the range of freedom in all dimensions equal. Therefore we will work towards a 3 dimensional harmonic oscillator in this thesis.

1.2. Laser optical trap

The laser optical trap is a set of lasers that have a frequency marginally lower than an exited state of the bosons. This means bosons with low impulse do not react with the lasers photons. However if a boson has an impulse opposite to that of the photons the energy difference means it can interact due to the Doppler Effect. Therefore it will absorb the photons impulse and therefore slow down. The boson itself will fall back to it ground orbit releasing a photon in a random direction. So photons are absorbed in the direction a boson is traveling in and ejected in a random direction. This will result in an decrease in impulse and therefore energy is decreased.

In order to decrease the energy of particles in all directions all three axis need lasers and they need to be pointed in both directions. These lasers do slow down particles in any direction, and therefore cools the gas down however it does not change with space therefore does not oppose diffusion. In order to get condensation the gas needs to be dense. This can be achieved with a magnetic trap.

1.3. Thesis overview

In this thesis we will go no further into the method of producing a BEC of positronium. The goal of this thesis is to describe the dynamics of such a system, where we generalize to a system with condensation and annihilating particles. To get to such a system we first need a model that properly describes a BEC and where we can introduce an annihilation therm. In chapter 5 we will describe BEC from a statistical physics background. Than we will build a Zero range process that has the same equilibrium properties as the statistical physics theory. Before we can do that we need to have a good understanding of the Zero range process.

In order to do this chapter 2 we will describe and explore a Markov process. We do this because the Zero range processes are a specific set of Markov processes. The theory of zero range processes is described in chapter 3. In chapter 4 we will introduce an annihilation therm to a zero range model with condensation on a single slow site. This single slow site zero range process is a rather simple system. Therefore we derive a differential equation that describes the number of particles at that site.

In chapter 6 we will first do some simulations to confirm that the zero range process in chapter 4 and the differential equation described there are the same in the large system limit. Than we derive an approximation of a system with energy levels like a 3D harmonic potential. We compare these results to those in [3], that we explored in chapter 5. In this same approximation we added an annihilation therm and see how the particles redistribute when annihilation is introduced.

2

Markov processes

In this chapter Markov processes are defined, and the properties of Markov processes are discussed. This is the mathematical foundation for the Zero Range process.

A stochastic process is a process which describes the random evolution of a system in the course of time. A stochastic process is called a Markov process if it has “no memory”. This means that conditioned on the current state of the process, the distribution of future states only depends on that current state, and not on the further past, i.e., not on how the current state has been reached. Equivalently, conditioned on the current state, the past and future of the process are independent.

A simple example of a Markov process (in discrete time) is a random walk where the “no memory” property comes from the fact that the individual steps of the walk are independent.

Example 2.0.1. *Take a discrete time unit step random walk with independent steps* $X(\mathrm{T}) \in \mathbb{Z}$ *at time* $\mathrm{T} \in \mathbb{N}$. *i.e.* $X(\mathrm{T}) = \sum_{i=1}^{\mathrm{T}} \xi_i$ *where* ξ_i *are all independent from one another and* $P(\xi_i = 1) = P(\xi_i = -1) = \frac{1}{2}$ *for all* i.

This is a mathematical model for a system of a particle on a grid. In this example, every second the particle has a 50% chance to hop one unit to the right and a 50% chance to hop one unit to the left (independent from one another). Now $X(\mathrm{T})$ *is the position of the particle.*

For this process one can calculate the probability distribution for the particle at any time. Also when we know that at a time T *the system is at place* $X(T)$. *We can calculate the probability distribution* $P(X(\tau) = L \mid X(T))$ *of the particle time* $\tau > T$. *Here* L *represents the place of the particle. If we add to this that at time* $S < T$ *the particle is at* $X(S)$ *this does not change the probability distribution which becomes:*

$$P(X(\tau) = L|X(T), X(S)) = P(X(\tau) = L|X(T)) \tag{2.1}$$

This shows that the process is a Markov process, as it does not depend on the 'past' (S) *when the 'present'* (T) *is known and we talk about the 'future'* τ, *and thus has no memory.*

It is important to realize that there is a correlation between $X(\tau)$ *and* $X(S)$. *This does not prohibit the process from being Markov. However there is no correlation between* $X(\tau)|X(T)$ *and* $X(S)|X(T)$.

This example 2.0.1 is in discrete time and in this thesis is included only to gain intuition about the Markov property. It has set times when it transitions from one state to another. The phenomena we want to analyze however are continuous in time. Therefore we need to explore continuous time Markov processes.

As will be shown later, the Markov property will require the probability for the state to remain the same through out a time interval to be exponentially decaying (as a function of the length of the interval).

The probability density to hop from a certain state A to another state B will be constant when the system is in state A. But as the probability to be in state A decreases exponentially so does the probability density to hop from state A to state B.

We will now define in more mathematical terms the Markov property and provide some elements of Markov process theory.

2.1. Definition of the Markov process

Let Ω denote the state space of the process $X_t, t \geq 0$. i.e. For all $t \geq 0$, X_t is a random variable with values in Ω ($P(X_t \in \Omega) = 1$). In this thesis Ω will always be a countable set, Therefore all functions on Ω are measurable.

Definition 2.1.1 (Markov process)**.** Take a random process with state space Ω (Ω is assumed to be equipped with a σ-algebra). Denote $\mathcal{F}_t$ to be the σ-algebra generated by the random variables X_s, $0 \leq s \leq t$

The process X_t, $t \geq 0$ is Markov if for every $f : \Omega \longrightarrow \mathbb{R}$.

$$\mathbb{E}(f(X_t)|\mathcal{F}_s) = \mathbb{E}(f(X_t)|X_s) \tag{2.2}$$

In this definition F_s is the σ-algebra generated by the state at all times before time s. This σ-algebra can be thought of as any subset of the history of the system. Therefore the Markov property can be interpreted as; the future of the system depends on the latest known state only, any information before that does not change the probability of the future in any way.

In this thesis the processes will have a discrete state space and will be continuous in time. For these state spaces, the process is uniquely determined by the transition probabilities.

$$P_t(x, y) = P(X_t|X_0 = x) = P(X_{s+t}|X_s = x) = P(X_{s+t}|X_s = x, X_{[0,s)}) \tag{2.3}$$

Where $X_{[0,s)}$ is any information about the state of the system in the time interval $[0, s)$.

2.1.1. Exponential waiting time

In this paragraph we will show how a Markov process with discrete state space and continuous time has a decaying probability to stay in one place. Here we notate $P(X_{[a,b]} = \alpha|Y) = P(X_t = \alpha \ \ \forall t \ \in [a, b]|Y)$.

Theorem 2.1.1. *Take a Markov process X_t, $t \geq 0$ with $X_t \in \Omega$ and $X_t = \alpha$. The probability for the system to be in state α trough out the interval $[t, t + s], s \geq 0$ is an exponential: $P(X_{[t,t+s]} = \alpha) = e^{-\lambda s}$. Where $\lambda > 0$ independent of time.*

Proof. Let us first show that $P(X_{[0,s]} = \alpha) = e^{-\lambda s}$. Here take λ to be the first therm in the Taylor expansion of the probability

$$P(X_t = \alpha|X_0 = \alpha) = 1 - \lambda t + \mathcal{O}(t^2) \tag{2.4}$$

Now

$$P(X_{[0,s]} = \alpha|X_0 = \alpha) = \lim_{n\longrightarrow\infty} P(X_{\frac{s}{n}} = \alpha, X_{\frac{2s}{n}} = \alpha, ..., X_{\frac{ns}{n}} = \alpha|X_0 = \alpha) \tag{2.5}$$

using 2.3 we get

$$P(X_{[0,s]} = \alpha|X_0 = \alpha) = \lim_{n\longrightarrow\infty} P(X_{\frac{s}{n}} = \alpha|X_0 = \alpha)^n \tag{2.6}$$

And using 2.4 with $t \longrightarrow 0$ we get

$$P(X_{[0,s]} = \alpha) = e^{-\lambda s} \tag{2.7}$$

Now because of 2.3 it must be true that $P(X_{[t,t+s]} = \alpha) = P(X_{[0,s]} = \alpha) = e^{-\lambda s}$ as all steps to prove 2.7 can be done with a time shift t. □

Example 2.1.1. *Consider a process which can take only two states A, B and flips between the two at random independent exponential times mean 1.*
This process is Markov because the transitions are independent from one another, and the exponential

distribution makes one transition independent from itself.

Let us calculate the probability distribution when $X_0 = A$.

Because we have only two states and identical transition probabilities we can use that the probability for the system to be in state A after time t is equal to the probability that the number of jumps is even, and the probability to be in state B is equal to the probability that the number of jumps is odd. We end up with a sum over a Poisson distribution.

$$P(X_t = A|X_0 = A) = P(\#transitions_{[0,t]} = even) = \sum_{k=0}^{\infty} \frac{t^{2k}}{2k!} e^{-t} = (\frac{e^{-t}}{2} + \frac{e^{t}}{2}) * e^{-t} = \frac{1}{2} + \frac{1}{2} e^{-2t} \quad (2.8)$$

To illustrate the difference between $P(X_t = \alpha)$ and $P(X_{[0,t]} = \alpha)$ for this example both are plotted in figure 2.1

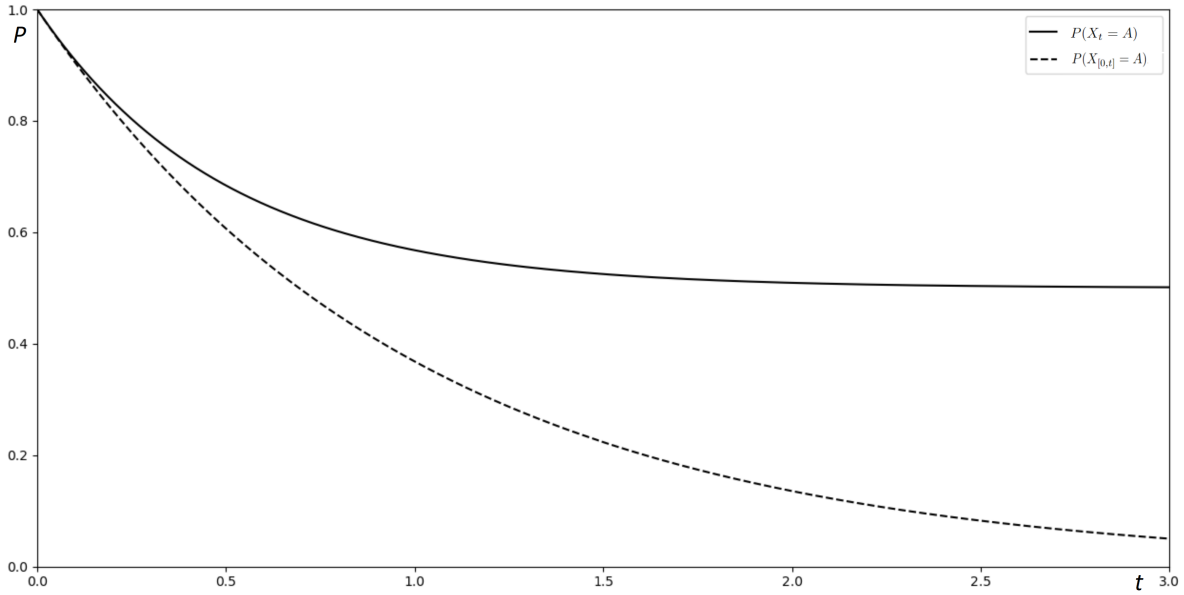


Figure 2.1: $P(X_t = A|X_0 = A)$ and $P(X_{[0,t]} = A|X_0 = A)$

It is clear that for small times the behaviour is similar. However when we include the chance to go from site A to B and back to A and even more hops back and forth the difference becomes larger when the time increases. This is because $P(X_{[0,t]} = A|X_0 = A)$ is the probability for no transitions to occur at all.

This behaviour can be expected in every Markov process. For very small timescales only one transition needs to be taken into account. However as the time increases the higher orders of transitions take over.

2.2. Chapman-Kolmogorov equation

All systems considered in this thesis have a countable state space and satisfy equation 2.3. Such systems can be uniquely described by their transition probabilities $P_t(x, y)$ defined by

$$P_t(x, y) = P(X_t = y|X_0 = x) = P(X_{t+s} = y|X_s = x) \quad (2.9)$$

where $x, y \in \Omega$.

Theorem 2.2.1. *These translation probabilities satisfy the Chapman-Kolmogorov equation 2.10*

$$P_{t+S}(x,y) = \sum_{z\in\Omega} P_t(x,z)P_s(z,y) \tag{2.10}$$

Proof.

$$P(X_{t+s} = y|X_0 = x) = \sum_{z\in\Omega} P(X_{t+s} = y, X_t = z|X_0 = x) = \sum_{z\in\Omega} P(X_{t+s} = y|X_t = z, X_0 = x)P(X_t = z|X_0 = x) \tag{2.11}$$

Now using that the process is Markov

$$P(X_{t+s} = y|X_0 = x) = \sum_{z\in\Omega} P(X_{t+s} = y|X_t = z)P(X_t = z|X_0 = x) \tag{2.12}$$

Using 2.3 we get

$$P(X_{t+s} = y|X_0 = x) = \sum_{z\in\Omega} P(X_s = y|X_0 = z)P(X_t = z|X_0 = x) = \sum_{z\in\Omega} P_s(z,y)P_t(x,z) \tag{2.13}$$

□

We can write these transition probabilities in a matrix, as we have countable state space and thus we can number the states in Ω as x_n, $n \in \mathbb{N}$.
For this the matrix P_t with values $P_t[a,b] = P_t(x_a, x_b)$. It is easy to see in matrix notation the Chapman-Kolmogorov equations can be written as

$$P_{t+s} = P_t P_s \tag{2.14}$$

2.2.1. Trajectories

We can also compute the probability of a finite trajectory to happen, (for $X_{t_1} = X_1$ and then $X_{t_2} = X_2$ and so on).

$$P(X_{t_1} = x_1, X_{t_2} = x_2, ..., X_{t_n} = x_n|X_{t_0} = x_0) = P_{t_1-t_0}(x_0,x_1)P_{t_2-t_1}(x_1,x_2)...P_{t_n-t_{n-1}}(x_{n-1},x_n) \tag{2.15}$$

Now using that all for continuous Markov processes equation 2.9 holds, we get

$$p(X_{t_n} = x_n|X_0 = x_0, X_1 = x_1, ..., X_{n-1} = x_{n-1}) = P(X_{t_n} = x_n|X_{t_{n-1}} = x_{n-1}) \tag{2.16}$$

This shows that for a set Chapman-Kolmogorov equations the corresponding random process is a Markov process. This is because for any possible history, the future only depends on the most recent known state.

2.3. Semigroups and generators

2.3.1. Semigroups

For any function $f : \Omega \to \mathbb{R}$ we can define an operator S_t such that:

$$S_t f(x) = \mathbb{E}(f(X_t)|X_0 = x) \tag{2.17}$$

Theorem 2.3.1. *This family of operators we call the semigroups $S_t, t \leq 0$. These have the following properties:*

1. $S_0 = I$ — *identity at $t = 0$*
2. $\lim_{\delta\downarrow 0} S_{t+\delta} = S_t$ — *right continuity*
3. $S_{t+s} = S_t S_s$ — *semigroup property*
4. $f \geq 0 \implies S_t f \geq 0$ — *positivity*
5. $S_t 1 = 1$ — *normalization*
6. $||s_t f(x)||_\infty = \sup_x |S_t f(x)| \leq \sup_x |f(x)|$ — *contraction*

Proof. (corresponds to numbers)
1.

$$S_0 f(x) = \mathbb{E}(f(X_0)|X_0 = x) = \mathbb{E}(f(x)) = f(x) \tag{2.18}$$

2. Take $Y, Z \in \Omega$. First we will show $\lim_{\delta \downarrow 0} P_\delta(Z, Y) = I$.
If $Y \neq Z$, $P_\delta(Z, Y) = \lambda * \delta = \mathcal{O}(\delta^2)$(because of exponential property). Thus $\lim_{\delta \downarrow 0} P_\delta(Z, Y) = 0$.
And similarly $P_\delta(Y, Y) = 1O(t)$
Thus $\lim_{\downarrow 0} P_\delta(Z, Y) = I$
Now to show right continuity

$$\lim_{\delta \downarrow 0} S_{t+\delta} f(x) = \lim_{\delta \downarrow 0} \mathbb{E}(f(X_{t+\delta})|X_0 = x) = \lim_{\delta \downarrow 0} \sum_{y \in \Omega} f(y) P_{t+\delta}(x, y) \tag{2.19}$$

$$= \lim_{\delta \downarrow 0} \sum_{y \in \Omega} f(y) \sum_{z \in \Omega} P_t(x, z) * P_\delta(z, y) = \sum_{y \in \Omega} f(y) \sum_{z \in \Omega} P_t(x, z) * \lim_{\delta \downarrow 0} P_\delta(z, y) = S_t f(x) \tag{2.20}$$

3. From Chapman-Kolmogorov

$$S_{t+s} f(x) = \sum_{y \in \Omega} P_{t+s}(x, y) f(y) = \sum_{y \in \Omega} \sum_{z \in \Omega} P_t(x, z) P_s(z, y) f(y) = S_t(S_s f(x)) \tag{2.21}$$

4. Take f such that $\forall x \in \Omega\ f(x) \geq 0$.

$$S_t f(x) = \mathbb{E}(f(X_t)|X_0 = x) = \sum_{y \in \Omega} P(X_t = y|X_0 = x) f(y) \tag{2.22}$$

Since $P(X_t = y|X_0 = x) \geq 0$ because it is a probability and we said $f(y) \geq 0$ we sum over positive things. Therefore it must be that $S_t f \geq 0$

5. Take $f(x) = 1$ for all $x \in \Omega$. Now for $y \in \Omega$, $S_t f(y) = \mathbb{E}(f(X_t)|X_0 = x) = 1$

6. Take $x \in \Omega$, $S_t f(x) = \mathbb{E}(f(X_t)|X_0 = x) = \sum_{y \in \Omega} P(X_t = y|X_0 = x) * f(y) \leq \sum_{y \in \Omega} P(X_t = y|X_0 = x) \sup_{x \in \Omega} |f(x)| = 1 * \sup_{x \in \Omega} |f(x)| = \sup_x \in \Omega |f(x)|$ □

If one has a space Ω, and $S_t, t \geq 0$ is a family of operators C(Ω) satisfying the 6 properties of semigroups. Then this is called a Markov semigroup. This corresponds to a Markov process with formula 2.17

Example 2.3.1. *In example 2.1.1 we calculated the probability to be in state A at time t given $X_0 = A$ (Noted as $P_t(A, A)$). From that we can easily determine $P_t(B, A) = 1 - P_t(A, A)$. We can also take $P_t(B, B) = P_t(A, A)$, as the problem is symmetric and $P_t(A, B) = 1 - P_t(B, B)$. With these transition probabilities we can determine the corresponding semigroup as a matrix.*

$$S_t = \begin{bmatrix} P_t(A, A) & P_t(B, A) \\ P_t(A, B) & P_t(B, B) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + e^{-2t} & 1 - e^{-2t} \\ 1 - e^{-2t} & 1 + e^{-2t} \end{bmatrix} \tag{2.23}$$

Take some function $f : \Omega \longrightarrow \mathbb{R}$. Now $S_t f(A) = \mathbb{E}(f(X_t)|X_0 = A) = P(X_t = A|X_0 = A) f(A) + P(X_t = B|X_0 = A) f(B)$. We can see this as we multiply S_t with the function f written in vector form. And we get

$$S_t f = \begin{bmatrix} P_t(A, A) & P_t(B, A) \\ P_t(A, B) & P_t(B, B) \end{bmatrix} \begin{bmatrix} f(A) \\ f(B) \end{bmatrix} = \begin{bmatrix} P_t(A, A) f(A) + P_t(B, A) f(B) \\ P_t(A, B) f(A) + P_t(B, B) f(B) \end{bmatrix} \tag{2.24}$$

which is a vector of semigroup values for different initial states.

2.3.2. Generator

In any random process the probability to transition form one state to another must depend on something. A Markov process this transition probability cannot depend on the state at any other time, therefore it must depend on the current state of the system and nothing else.

This dependency will be modeled using generator L. The change in state can be interpreted as the rate of change of the system, and therefore as the small time limit of semigroup over the time. Like a ”derivative” of a random process. The generator is defined as

Definition 2.3.1. For some semigroup S_t define L such that

$$Lf(x) = \lim_{t\to 0} \frac{S_t f(x) - f(x)}{t} = \lim_{t\to 0} \frac{f(x+t) - f(x)}{t} \tag{2.25}$$

and therefore we get L itself is

$$L = \lim_{t\to 0} \frac{S_t f - f}{t} \tag{2.26}$$

2.3.3. Properties of the generator

Presume L to be a $\#\Omega$ by $\#\Omega$ matrix. The diagonal must contain only numbers ≤ 0. Anything of diagonal must be ≥ 0. (both obvious when multiply with the corresponding state) also the columns must sum to 0. (in order for the system to be found in 1 state at a time).

If these properties are met the generator can be reversed to semigroup with all the properties associated with 2.17. And therefore be reversed to a unique Markov process.

Proof. Take L a square matrix with columns sum to 0 and non-positive diagonal values, non-negative other values. Take $S_t = e^{tL}$, clearly this semigroup is uniquely defined by L. Also $lim_{t\to 0}\frac{S_t f - f}{t} = L$. Now to the propperties:
1. $S_0 = e^0 = I$
2. e^{tL} is a right continuous function
3. $e^{(t+s)L} = e^{tL} * e^{sL}$
4. tr$(-tL) \geq 0 \longrightarrow \det e^{-tL} > 0)$
5. $e^{tL}1 =$ columns L sum to 0 thus S to 1? thus normalization
6. $e^{-tL}f(x) =$ ....

□

2.3.4. Transition rates and generators

The generator can be interpreted as the change in state. However if we want to look into specific states and how they change we do not need information about all the states. We can also just look at the speed from one specific state to another. Therefore we introduce the transition rates.

Definition 2.3.2 (transition rates)**.** The transition rate from state $\eta \in \Omega$ to state $\xi \in \Omega$ for $\eta \neq y$ is defined as.

$$c(\eta, \xi) = \lim_{t\to 0} \frac{P(X_t = \xi | X_0 = \eta)}{t} \tag{2.27}$$

And it is easy to see that.

$$Lf(\eta) = \sum_{y\epsilon\Omega} (c(\eta, \xi)(f(\xi) - f(\eta)) \tag{2.28}$$

Example 2.3.2. *Take 2.3.2. Now we want to calculate the transition rates.*

$$c(A, B) = \lim_{t\to} \frac{1 - e^{-2t}}{2t} = 1 \tag{2.29}$$

$$c(B, A) = \lim_{t\to} \frac{1 + e^{-2t}}{2t} = 1 \tag{2.30}$$

In this case $L = \begin{bmatrix} -\sum_{\alpha\neq A} c(A,\alpha) & c(B,A) \\ c(A,B) & -\sum_{\beta\neq B} c(B,\beta) \end{bmatrix} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$

2.4. Invariant measures

In this section first the concept of a stationary measure is introduced. Later a formal definition will be shown. In the end the concept of Detailed balance will be introduced.

Example 2.4.1. *In 2.3.2 it is clear we get to an equilibrium since from whatever state we start, whatever* $f : \Omega \longrightarrow \mathbb{R}$ *we take, for* $t \longrightarrow \infty$ *we get*

$$\mathbb{E}(f(X_t)) = \frac{c(A,B) * f(B) + c(B,A) * f(A)}{c(A,B) + c(B,A)} \tag{2.31}$$

This means that the probability for the system to be in state A *is constant, and equal to* $\frac{C(B,A)}{c(A,b)+C(B,A)}$.

Definition 2.4.1. Take a Markov process on a measurable compact space Ω, and a semigroup $St, t > 0$ corresponding to the Markov process. Take μ a probability measure on Ω, μ is an invariant measure if for all $f \epsilon C(\Omega)$, $\forall t \geq 0$

$$\int S_t f d\mu = \int f d\mu \tag{2.32}$$

If now 2.3.1 is applied to a probability measure we get

$$\int L f d\mu = 0 \tag{2.33}$$

For Ω countable it is possible to write S_t and L as linear operators on μ. In that case the integral can be replaced with a sum.

$$\sum_{\eta \epsilon \Omega} S_t f(\eta) \mu_\eta = \sum_{\eta \epsilon \Omega} f(\eta) \mu_\eta \tag{2.34}$$

And thus μ can be interpreted as a vector corresponding to a probability for all states of Ω to be in when the system is in equilibrium. So if the system stabilizes after a certain time the resulting distribution is a stationary measure

The generator can also be calculated, we get for countable Ω because the intergral over a finite space can be replaced with a sum we get

$$\sum_{\eta \epsilon \Omega} (L)_{\eta,\xi} f(\xi) \mu(\eta) = 0 \tag{2.35}$$

Since $f(\xi)$ can be any function with $f : \Omega \longrightarrow \mathbb{R}$ it must be true that

$$\sum_{\eta \epsilon \Omega} (L)_{\eta,\xi} \mu(\eta) = 0 \tag{2.36}$$

And thus we can write this as a matrix multiplication.

$$\bar{\mu} * L = \bar{0} \tag{2.37}$$

The fact that the semigroup action on the stationary measure results in the stationary measure, can be interpreted as the stationary measure does not change when the Markov process works on it.

Similarly the generator acting on the stationary measure results in a zero vector or integral. Because of the definition 2.3.1 the generator can be tough of similar as the derivative but for a random process.

A Markov process homogeneous in time has a similar link to a first order homogeneous differential equation. However we still do not talk about deterministic values but about probabilistic densities.

2.4.1. Detailed balance

In this subsection a more specific set of stationary measures will be explored. First reversibility will be defined, and see it is equivalent to a system in detailed balance. Than a proof that a system in detailed balance is a system in a stationary measure. Than the Markov processes that have a stationary measure that is also in detailed balance will be explored.

Definition 2.4.2 (Reversibility)**.** A probability measure μ is in reversible if $\forall f, g$, $\forall t \geq 0$

$$\sum_{\eta} \mu(\eta) S_t f(\eta) g(\eta) = \sum_{\eta} \mu(\eta) S_t(g(\eta)) f(\eta) \tag{2.38}$$

or equivalent is

$$\sum Lf(\eta) g(\eta) \mu(\eta) = \sum g(\eta) Lf(\eta) \mu(\eta \tag{2.39}$$

The generator is self adjunct in $L^2(\mu)$
If we will in $f = \delta_{\eta,\xi}$ and $g = \delta_{\xi,\eta}$ we get

$$\mu(\eta) c(\eta, \xi) = \mu(\xi) c(\xi, \eta) \tag{2.40}$$

This we call detailed balance.

Theorem 2.4.1. *If μ is reversible, μ is a stationary measure*

Proof. Take μ reversible, thus $\mu(\eta)c(\eta,\xi) = \mu(\xi)c(\xi,\eta)$. Because a stationary measure is equivalent to a generator action on the measure equal to zero proving $\bar{\mu} * L = 0$ is enough. Take any $\xi \epsilon \Omega$ now calculate $\sum_{\eta \epsilon \Omega} (L)_{\eta,\xi} \mu(\eta)$. It is known that $(L)_{\xi,\xi} = -\sum_{x \epsilon \Omega \setminus \{\xi\}} c(\xi, x) \mu(\xi)$ but because for $x \neq y$ $(L)_{x,y} = c(x,y)$ we get:

$$\begin{aligned} \sum_{\eta \epsilon \Omega} (L)_{\eta,\xi} \mu(\eta) = \sum_{\eta \epsilon \Omega \setminus \{\xi\}} (L)_{\eta,\xi} \mu(\eta) + (L)_{\xi,\xi} &= \sum_{\eta \epsilon \Omega \setminus \{\xi\}} c(\eta, \xi) \mu(\eta) - \sum_{\eta \epsilon \Omega \setminus \{\xi\}} c(\xi, \eta) \mu(\xi) \\ &= \sum_{\eta \epsilon \Omega \setminus \{\xi\}} c(\eta, \xi) \mu(\eta) - c(\xi, \eta) \mu(\xi) = \sum_{\eta \epsilon \Omega \setminus \{\xi\}} 0 = 0 \end{aligned} \tag{2.41}$$

This is independent in ξ thus $\bar{\mu} * L = 0$ □

Thus a reversible measure is always stationary, but a stationary measure is not necessarily reversible.

Example 2.4.2. *Take a random process with $\Omega = \{A, B, C\}$ and $L = \begin{bmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$ $\mu = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix}$ is a stationary measure as $L\mu = 0$ but $\mu(A)L(A,B) = \frac{1}{3} \neq 0 = \mu(B)L(B,A)$ Thus μ is a stationary measure but not in detailed balance.*

3

Zero-range process

In this section the zero range process introduced. This is based on [1]. Later some aspects of statistical physics will be compared to the properties of the zero range process.

In [1] a system is described as a set of particles and a set of sites. We will use the therm state as one distribution of particles over the sites. This means when we have finite particles n and sites l the number of states $\#\Omega = \binom{n+l}{l}$. A zero range process will be a Markov process with this many states. However the number of states grows fast compared to the number of sites and particles

3.1. Introduction Zero-range process

Before we formalize the Zero-range process let us visualize what it is.

Example 3.1.1. *Let us take a system with 10 sites and 12 particles. A possible distribution of these particles is represented in 6.1. Here the sites are numbered* $0, 1, \ldots, 9$ *and the particles are represented as a circle.*

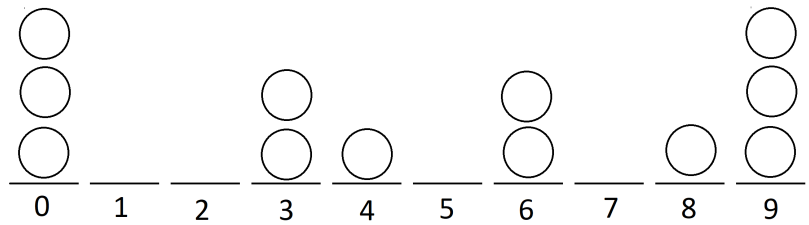


Figure 3.1: Example of particles at sites

In this state the number of particles at site 0 *is 3, the number of particles at site* 1 *is 0, and so on.*

As we assume the particles to be indistinguishable. Now if we know how many particles there are at each site we know everything there is to know about the system. Therefore we can describe the

state as

$$\eta = \begin{bmatrix} 3 \\ 0 \\ 0 \\ 2 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \\ 3 \end{bmatrix} \tag{3.1}$$

The values of this vector must be natural numbers as it is not possible to find half a particle in a state. Now one particles hops from site 3 to site 2. Now after this hop the system is in state η' as this is

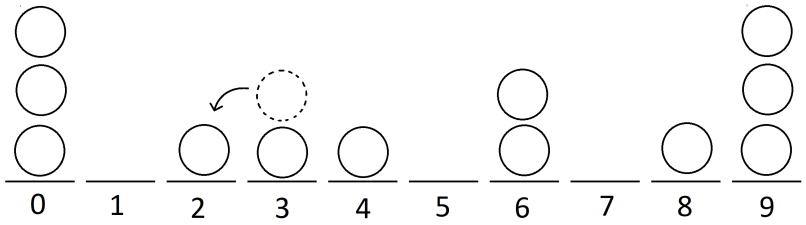


Figure 3.2: One particle hops from site 3 to site 2

equal to state η but with where one particle hopped from state 3 to state 2 we notate $\eta' = \eta^{3,2}$

$$\eta' = \eta^{3,2} = \begin{bmatrix} 3 \\ 0 \\ 0+1 \\ 2-1 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 2 \\ 0 \\ 1 \\ 3 \end{bmatrix} \tag{3.2}$$

Now for the system to be Zero-range, it must be true that the rate to hop from site i to site j only depends on the number of particles at site i, which is notated as η_i. Thus

$$c(\eta, \eta^{i,j}) = C_{i,j}(\eta_i) \tag{3.3}$$

And in this example $i = 3$ and $j = 2$ and thus the rate to go from site 3 to site 2 only depends on the number of particles at site 3.

Definition 3.1.1. A Zero range process is a Markov process where $\Omega = \mathbb{N}_0^L$ where $L \in \mathbb{N} \cup \infty$ Now the transition rates are

$$c(\eta, \eta^{i,j}) = C_{i,j}(\eta_i) \tag{3.4}$$

and if there exist no $i, j \in \{0, 1, ..., L-1\}$ such that $\eta_{i,j} = \xi$ the rate $c(\eta, \xi) = 0$.

Example 3.1.2. *Take a system with 2 particles in 2 sites (site 0 and site 1. The possible states are $\left\{\begin{bmatrix}2\\0\end{bmatrix}, \begin{bmatrix}1\\1\end{bmatrix}, \begin{bmatrix}0\\2\end{bmatrix}\right\}$ If the system is a Zero range process, the rate $c\left(\begin{bmatrix}2\\0\end{bmatrix}, \begin{bmatrix}0\\2\end{bmatrix}\right) = 0$ because there is no direct transition between the two.*

If we take $C_{0,1}(n) = C_{1,0}(n) = n$ *we can calculate all the transition rates:*

$$c\left(\begin{bmatrix}2\\0\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix}\right) = c\left(\begin{bmatrix}0\\2\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix}\right) = 2 \tag{3.5}$$

$$c\left(\begin{bmatrix}1\\1\end{bmatrix},\begin{bmatrix}2\\0\end{bmatrix}\right) = c\left(\begin{bmatrix}1\\1\end{bmatrix},\begin{bmatrix}0\\2\end{bmatrix}\right) = 1 \tag{3.6}$$

The process is in detailed balance for $\mu\left(\begin{bmatrix}2\\0\end{bmatrix}\right) = \mu\left(\begin{bmatrix}0\\2\end{bmatrix}\right) = \frac{1}{4}$ *and* $\mu\left(\begin{bmatrix}1\\1\end{bmatrix}\right) = \frac{1}{2}$

Example 3.1.3. *Take the same system as 3.1.2 but now* $C_{0,1}(n) = c_{1,0}(n) = c\mathbb{1}_{>0}(n)$*, where* $\mathbb{1}_{>0}(n)$ *the indicator function equal to* 1 *if* $n > 0$*,* 0 *otherwise. Now*

$$c\left(\begin{bmatrix}2\\0\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix}\right) = c\left(\begin{bmatrix}0\\2\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix}\right) = c\left(\begin{bmatrix}1\\1\end{bmatrix},\begin{bmatrix}2\\0\end{bmatrix}\right) = c\left(\begin{bmatrix}1\\1\end{bmatrix},\begin{bmatrix}0\\2\end{bmatrix}\right) = c \tag{3.7}$$

This process is in detailed balance for $\mu\left(\begin{bmatrix}2\\0\end{bmatrix}\right) = \mu\left(\begin{bmatrix}1\\1\end{bmatrix}\right) = \mu\left(\begin{bmatrix}0\\2\end{bmatrix}\right) = \frac{1}{3}$

Because for a lot of Zero-range systems the number of states grows fast with system size (more than exponentially). We want to find a way to compute the expected number of particles at sites without the need to compute the invariant measures.

3.2. Grand canonical reversible product measures

One of the most use full characteristics of Zero-range processes is that when the transition rates can be written as 3.8 the stationary measure can be constructed as a product of factors that only dependent on one site each. i.e, it is a product measure.

$$c(\eta, \eta^{i,j}) = C_{i,j}(\eta_i) = W_{i,j}u_i(\eta_i) \tag{3.8}$$

Note that $W_{i,j}$ does not depend on η_i. This is a necessary if we want to write the stationary measure as a product.

Example 3.2.1. *Take zero range process with sites* $\{0, 1, \ldots, L\}$ *and with* $W_{i,j} = \frac{1}{L}$ *for* $i \neq j$*.*
Now two possible distributions of N *particles,* $\eta, \eta^{i,j}$ *where* $\eta_i = \eta_i^{i,j} - 1$ *and* $\eta_j = \eta_j^{i,j} + 1$ *and at all other sites they are equal. Now say* $\mu : \Omega \longrightarrow \mathbb{R}$ *is an invariant measure. Now tor any* $f : \Omega \longrightarrow \mathbb{R}$

$$\sum_{\eta'} W_{i,j}u_i(\eta_i)f(\eta)\mu(\eta^{i,j}) = 0 \tag{3.9}$$

because all other factors of L *must be zero as it is a zero range process. Because of our simplified* W *we get to the equation*

$$\frac{\sum_{i\neq j} u_i(\eta_i)\mu(\eta^{i,j})}{L} = u_j(\eta_j) \tag{3.10}$$

For every site i of the process there is a function $f_i(\eta_i)$, where η_i is the number of particles at site i when the system is in state η.

$$\mu(\eta) = \frac{\prod_{i\in\mathbb{L}} f_i(\eta_i)}{\sum_{\eta\in\Omega}\prod_{i\in\mathbb{L}} f_i(\eta_i)} \tag{3.11}$$

where $\mathbb{L}$ is the set of sites of the system.

In Example 3.11 the denominator is simply to normalize μ because it is a probability measure and therefore must sum to one.

If we take

$$f_i(\eta_i) = \prod_{k=1}^{\eta_i} \left[\frac{s_i}{u_i(k)} \right] \tag{3.12}$$

where s_i is such that

$$s_i = \sum_{j \in \mathbb{L}} s_j W_{i,j} \tag{3.13}$$

Where $u_i(\eta_i) = \sum_{j \neq i} C_{i,j}(\eta_i)$, and $W_{i,j}(\eta_i) = \frac{C_{i,j}(\eta_i)}{u_i(\eta_i)}$
.
From now on all systems considered will have $W_{i,j}(\eta_i) = W_{j,i}(\eta_j)$. This means the distribution of particles leaving site i only depends on the number of particles at site i.

Theorem 3.2.1. *The measure in detailed balance can be written as* $\mu(\eta) = \prod_i \mu_i(\eta_i)$ *with* $\mu_i(n) = \frac{z^n}{\Psi_i(z) \prod_{k=1}^n u_i(k)}$ *and* $\Psi_i(C) \sum_{n=0}^{\infty} \frac{C^n}{\prod_{k=1}^n}$

Proof. Take $\mu(\eta)$ to be a probability measure in detailed balance. Now it must be true that for $\eta, \xi \in \Omega$ if $\eta_i = \xi_i$ that $\frac{\mu(\eta)}{\mu(\eta^{i,j})} = \frac{\mu(\xi)}{\mu(\xi^{i,j})}$ because these two must have the same rate to one another. Therefore the detailed balance must have the same difference in probability.

This property goes for every site. Therefore we can introduce a product measure, such that

$$\mu(\eta) = \prod_{i=0}^{L} \mu_i(\eta_i) \tag{3.14}$$

Now because of reversibility

$$c(\eta, \eta')\mu(\eta) = c(\eta', \eta)\mu(\eta') \tag{3.15}$$

this is a zero range system so the only rates that are none-zero correspond to a hop from one site to another. Thus we can write

$$c(\eta, \eta^{i,j})\mu(\eta) = c(\eta^{i,j}, \eta)\mu(\eta^{i,j}) \tag{3.16}$$

and thus

$$W_{i,j} u(\eta_i)\mu(\eta) = W_{j,i} u(\eta_j + 1)\mu(\eta^{i,j}) \tag{3.17}$$

And if we fill in $W_{i,j} = W_{j,i}$ we get

$$u_i(\eta_i) \prod_{k=0}^{L} \mu_k(\eta_k) = u_j(\eta_j + 1) \prod_{k=0}^{L} \mu_k(\eta_k^{i,j}) \tag{3.18}$$

These products have all but the terms i, j in common. The equation can be divided by all the other therms.

$$u_i(\eta_i) * \mu_i(\eta_i)\mu_j(\eta_j) = u_j(\eta_j + 1)\mu_i(\eta_i - 1)\mu_j(\eta_j + 1) \tag{3.19}$$

Now take all therms depending on η_i to the left side of the equation and all therms depending on η_j to the right side of the equation.

$$\frac{u_i(\eta_i)\mu_i(\eta_i)}{\mu_i(\eta_i - 1)} = \frac{u_j(\eta_j + 1)\mu_j(\eta_j + 1)}{\mu_j(\eta_j)} \tag{3.20}$$

Because both sides of this equation strictly depend on different variables they must be equal to a constant C.

$$\frac{\mu_i(\eta_i)}{\mu_i(\eta_i - 1)} = \frac{C}{u_i(\eta_i)} \tag{3.21}$$

This must be true for all sites i. Therefore in a stationary measure all sites must obey this equation with the same constant C. With this value we now can calculate the values for μ_i using equation 3.21 n times we get

$$\mu_i(n) = \frac{C^n}{\prod_{k=1}^{n} u_i(k)} \mu_i(0) \tag{3.22}$$

but because μ_i is a probability measure, all possible μ_i must be equal to one.

$$\sum_{k=0}^{\infty} \mu_i(k) = 1 \tag{3.23}$$

thus

$$\mu_i(0) \sum_{n=0}^{\infty} \frac{C^n}{\prod_{k=1}^{n} u_i(k)} = 1 \tag{3.24}$$

Now take $\mu_i(0) = \frac{1}{\Psi_i(C)}$ and we get

$$\Psi_i(C) = \sum_{n=0}^{\infty} \frac{C^n}{\prod_{k=1}^{n} u_i(k)} \tag{3.25}$$

$\Psi_i(c)$ is used as the normalisation of the probability measure. □

Now because this C is constant over all sites, the stationary measure over all can be calculated. The probability measure over different sites only depend on C therefore the combination is a multiplication over the sites.

$$\mu(\eta) = \prod_i \mu_i(\eta_i) \tag{3.26}$$

where

$$\mu_i(n) = \frac{z^n}{\prod_{k=1}^{n} u_i(k)} \frac{1}{\Psi_i(z)} \tag{3.27}$$

Now taking $z = C$ because it is a 'constant' for all sites. But now it is a choice thus a variable.

Example 3.2.2. *Take a Zero range system where for all sites $u_i(n) = n$ and also assume uniform redistribution. Now calculate $\Psi(z)$*

$$\Psi_i(z) = \sum_{n=0}^{\infty} \frac{z^n}{\prod_{k=1}^{n} k} = \sum_{n=0}^{\infty} \frac{z^n}{n!} = e^z \tag{3.28}$$

Now calculating $\mu_i(n)$

$$\mu_i(n) = \frac{z^n}{\prod_{k=1}^{n} k} e^{-z} = \frac{z^n}{n!} e^{-z} \tag{3.29}$$

And thus μ_i is Poisson distributed.

Example 3.2.3. *Take the same system as 3.2.2 but with $u_i(n) = c_i n$.*

$$\Psi_i(z) = \sum_{n=0}^{\infty} \frac{z^n}{c_i^n z!} = e^{\frac{z}{c_i}} \tag{3.30}$$

$$\mu_i(n) = \frac{z^n}{c_i^n n} e^{-\frac{z}{c_i}} \tag{3.31}$$

This is similar to the example 3.2.2 but now c_i can change for different sites. Thus in this case different rates from sites do not change the sort of distribution of one site

Example 3.2.4 (Homogeneous geometric)**.** *Take a zero range system but now all sites have rates* $\mu_i(n) = \mathbb{1}(n > 0)$ *the indicator function.*

$$\psi_i(z) = \sum_{n=0}^{\infty} \frac{z^n}{1} = \frac{1}{1-z} \quad \textit{for} \quad 0 < z < 1 \tag{3.32}$$

and thus we get

$$\mu_i(n) = z^n * (1 - z) \tag{3.33}$$

Example 3.2.5 (Homogeneous geometric with a single slow site)**.** *Take the same system as 3.2.4 but now take* $u_0(n) = c\mathbb{1}(n > 0)$ *where* $0 < c < 1$*. Now* μ_i *for* $i > 0$ *is the same as 3.2.4 thus only calculate* $\mu_0(n)$

$$\Psi_0(z) = \frac{z^n}{c^n} = \frac{1}{1 - \frac{z}{c}} \quad \textit{for} \quad 0 < z < c \tag{3.34}$$

$$\mu_0(n) = \left(\frac{z}{c}\right)^n (1 - \frac{z}{c}) \quad \textit{for} \quad 0 < z < c \tag{3.35}$$

Now we have different restrictions for the value of z*. Because* z *is the same for the entire system when in equilibrium,* z *must satisfy all restrictions put on it. In the next section this will be talked about more.*

3.2.1. Grand canonical ensemble

If one takes the sites as individual distributions and prescribe a z for the entire system the total distribution function is known as the grand canonical distribution function. However as the grand canonical distribution will be used for large systems the one does not introduce the number of sites and the number of particles, but rather the density of particles.

$$\mu_z(\eta) = \frac{\prod_{i=1}^{N} \Psi_i(z)}{\mathcal{Z}_z} \tag{3.36}$$

where

$$\mathcal{Z}_z = \sum_{\eta} \prod_{i=1}^{N} \Psi_i(z) \tag{3.37}$$

This distribution is known as the grand canonical ensemble. This distribution does not limit the number of particles in the total system. The relative likely hood for the system to be in a state with a set number of particles is right however. The next section is about correcting this.

3.3. The canonical invariant measure

The Grand canonical ensemble does not require the number of particles to be set. Whereas the zero range process does require the number of particles to be fixed. To make this clear we start with an example.

Example 3.3.1. *we start with the system as in 3.1.3, we calculate the distribution according to the grand canonical ensemble and the canonical ensemble.*

$$\mu_i(n) = z^n * 1 - z \tag{3.38}$$

for $i = 0, 1$ *Now we need to chose* z *such that* $\sum_{i=0,1} \sum_{n=1}^{\infty} n * \mu_i(n) = 2$*.*

$$\sum_{i=0,1} \sum_{n=1}^{\infty} n * \mu_i(n) = 2 * \frac{z}{1-z} \tag{3.39}$$

This is equal to 2 *for* $z = \frac{1}{2}$

Now notice that the probability to be in $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ *is* $\prod_{i=1,2} \mu_i(0) = \frac{1}{2} * \frac{1}{2} = \frac{1}{4}$*. This is becouse the Grand canonical ensemble does not constrain the number of particles.*

The number of particles cannot change. But the product measures are correct but we need to make sure the only states taken into account are those with the correct number of particles.

This distribution will be called ν.

$$\nu_{L,N}\left(\eta \mid \sum_{i=0}^{L}\eta_i = N\right) = \frac{\prod_i \mu_i(\eta_i) * \mathbb{1}(\sum_{1=0}^{L}\eta_i = N)}{\sum_{\eta':\sum_i \eta_i' = N}\prod_i \mu_i(\eta_i)} \tag{3.40}$$

Thus when the only valid configurations have exactly N particles, simply take those distributions and normalize only counting those.

Now fill in $\mu_i(n)$ from 3.27 and we get

$$\nu_{L,N}\left(\eta \mid \sum_{i=0}^{L}\eta_i = N\right) = \frac{\prod_i \frac{z^{\eta_i}}{\prod_{i=1}^{\eta_i} u_i(k)}\frac{1}{\Psi_i(z)}\ \ \mathbb{1}(\sum_{1=0}^{L}\eta_i = N)}{\sum_{\eta':\sum_i \eta_i' = N}\prod_i \frac{z^{\eta_i'}}{\prod_{i=1}^{\eta_i'} u_i(k)}\frac{1}{\Psi_i(z)}} \tag{3.41}$$

In order to simplify this take

$$H_i(n) = \prod_{j=1}^{n} u_i(j) \tag{3.42}$$

and we get

$$\nu_{L,N}\left(\eta \mid \sum_{i=0}^{L}\eta_i = N\right) = \frac{\mathbb{1}(\sum_{1=0}^{L}\eta_i = N)\prod_i \frac{1}{H_i(\eta_i)}}{\sum_{\eta':\sum_i \eta_i' = N}\prod_i \frac{1}{H_i(\eta_i')}} \tag{3.43}$$

Now the canonical ensemble $Z_{L,N}$ is defined as

$$Z_{L,N} = \sum_{\eta':\sum_i \eta_i' = N}\prod_i \frac{1}{H_i(\eta_i')} \tag{3.44}$$

and the canonical invariant measure $\nu_{L,N}(\eta)$ is

$$\nu_{L,N}(\eta) = \frac{\mathbb{1}(\sum_{1=0}^{L}\eta_i = N)\prod_i \frac{1}{H_i(\eta_i)}}{Z_{L,N}} \tag{3.45}$$

Example 3.3.2. *We will compute $\nu_{L,N}$ from example 3.3.1. In this case $L = 2$ and $N = 2$. First we need to compute $Z_{2,2}$. In order to do this we need to determine all states of the system η, such that $\sum_i \eta_i = N$. In this case* $\left\{\begin{bmatrix}2\\0\end{bmatrix}, \begin{bmatrix}1\\1\end{bmatrix}, \begin{bmatrix}0\\2\end{bmatrix}\right\}$.

$$Z_{2,2} = \sum_{\eta=\begin{bmatrix}2\\0\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix},\begin{bmatrix}0\\2\end{bmatrix}}\prod_{i=0,1}\frac{1}{\prod_{j=1}^{n} u_i(j)} = \sum_{\eta=\begin{bmatrix}2\\0\end{bmatrix},\begin{bmatrix}1\\1\end{bmatrix},\begin{bmatrix}0\\2\end{bmatrix}}\frac{1}{c^2} = \frac{3}{c^2} \tag{3.46}$$

now $\nu_{L,N}(\eta) = \frac{1}{3}$ for $\eta \in \left\{\begin{bmatrix}2\\0\end{bmatrix}, \begin{bmatrix}1\\1\end{bmatrix}, \begin{bmatrix}0\\2\end{bmatrix}\right\}$ just like example 3.1.3.

3.4. Particle density under grand Canonical ensemble

The density of particles ρ can be easily determined for the canonical distribution $\rho = \frac{N}{L}$. The grand canonical ensemble only has the factor z determining the density of particles. Here we calculate the relation between the density of particles and z for the system as in example 3.2.5.

$$\mu_z(\eta) = \prod_i \mu_i(\eta_i) = \prod_i \frac{z^{\eta_i}}{H_i(\eta_i)\Psi_i(z)} \tag{3.47}$$

here the expected number of particles at one site is

$$\mathbb{E}_{\mu_z}(\eta_i) = \sum_{n=0}^{\infty} n \frac{z^n}{H_i(n)\Psi_i(z)} = \frac{z\Psi_i'(z)}{\Psi_i(z)} \tag{3.48}$$

where Ψ_i is

$$\Psi_i(z) = \sum_{n=0}^{\infty} \frac{z^n}{H_i(n)} \tag{3.49}$$

Because we have only a single slow site and all other sites are equal we can presume as $L \longrightarrow \infty$ the single slow site does not influence the average density. (unless the number of particles in that site also grows to infinity). Therefore

$$\rho = \mathbb{E}[\mu_i(\eta_i)] \tag{3.50}$$

Now to calculate the expectation of the total number of particles in the system per state $\mathbb{E}_{\mu_z}(\frac{1}{L}\sum_{i=1}^{L}\eta_i)$. Here the slow site is not taken into account. This is because later the limit for large systems will be made, and therefore one site will be insignificant.

$$\rho = \mathbb{E}_{\mu_z}(\frac{1}{L}\sum_{i=1}^{L}\eta_i) = \frac{1}{L}\sum_{i=1}^{L}\frac{z\Psi_i'(z)}{\Psi_i(z)} \quad \text{for} \quad z = z(\rho) \tag{3.51}$$

Now using that all sites that are not the slow site are equal, thus

$$\Psi_i(z) = \Psi_j(z) = \Psi_1(z) \quad \text{for} \quad i,j\epsilon\{1,2,\ldots,L\} \tag{3.52}$$

However in examples 3.2.5 we see that there can be restrictions on z.
Now define $\rho_L(z)$ like

$$\mathbb{E}_{\mu_z}(\frac{1}{L}\sum_{i=1}^{L}\eta_i) = \rho_L(z) \tag{3.53}$$

Thus ρ is the average number of particles in sites $1,2,\ldots,L$ also

$$\lim_{L\longrightarrow\infty}\rho_L(z) = \rho(z) \tag{3.54}$$

$$\rho(z_c) = \rho_c \tag{3.55}$$

where $z_c = \sup\{z \quad \text{such that} \quad \forall i\epsilon\{0,1,\ldots,L\},\ \Psi_i(z) \text{ is a valid function}\}$.

3.4.1. Equivalence of ensembles

Since both μ_z and $\nu_{L,N}$ are the same size and use the same reversible product measures we would expect them to be similar if the expected number of particles is the same. The difference between the ensembles is the normalization. The canonical ensemble normalizes the total number of particles where the grand canonical ensemble normalizes the expectation value of all sites. (we set z such that the total expected number of particles is correct).

That would mean that for a zero range process the grand canonical distribution μ_z for z such that $\rho = \frac{N}{L}$ and canonical distribution $\nu_{L,N}$ for any site i are equivalent if $P_{\mu_z}[\eta_i = n] = P_{\nu_{L,N}}[\eta_i = n]$. For $n \in \mathbb{N}$.

The canonical and grand canonical ensemble are equivalent if $\forall i \lim_{N\longrightarrow\infty}\frac{\mathbb{E}_{\mu_z}[\eta_i]}{N} = 0$

We will not prove this statement, but we can see how this works. We have the reversible product measures those are constructed such that when the inflow of particles to a site is constant these becomes the probability density function for that site.

When we have a site that has a substantial part of the total particles the number of particles at that site influences the number of particles that can hop to other sites. The canonical ensemble compensates for this by only taking the states that have the correct number of particles. When the number of particles at any site cannot change that of the others because the expected number of particles at that site compared to the total is insignificant the canonical ensemble does nothing else than the grand canonical ensemble.

For a lot of system this means that for an infinite system size the grand canonical and canonical ensemble have the same distribution if z is such that $\rho(z) = \frac{N}{L}$. This however is not for all zero range systems the case. It is possible that when ρ increases there is one site that gets infinite particles. Here condensation occurs. We call the lowest density such that condensation happens ρ_0.

For systems where the hopping rates are equal for all non zero occupations, for $N \longrightarrow \infty$ we can set for $\rho > \rho_0$ that the equilibrium distribution is the grand canonical ensemble for z such that $\rho = \rho_0$ thus $\mu_{z(\rho_0)}$. Where all the other particles are at the condensed site such that the total density ρ is satisfied.

4

Single slow site

This thesis is about the change in properties of a Bose-Einstein condensate when at random particles are removed from the system. In this chapter a very specific zero range model is used to get a grip on the action of annihilating particles in a condensate.

4.1. Single-Slow site with uniform rates

Take a zero range process with uniform rates. Thus all have rate $u_j = 1$, and jump to a uniformly chosen target site. At site 0 the rate will be $c > 0$.

Now for $0 < c < 1$ we get a system where all rates are equal those leaving one specific site. That is the slow site.

Intuitively one could understand that condensation occurs when the number of particles becomes large with the following reasoning;
If more particles get into the system the average number of particles per site should rise. Therefore the rate at which particles hop from one site to another should rise.
Because all sites get particles at the same rate in order to be in equilibrium they need to leave all at the same rate.
However the sites have a maximum rate at which they lose particles this is $c < 1$ for the slow site, and 1 for all other sites. There is one site that reaches its limit of departing particles first, the slow site. At that point all particles added to the system will get into this site. This is because if other particles get higher occupation the rate departing these sites rises and therefore rate to slow site rises, and the system is not yet in equilibrium.

Now to make this idea more formal:

Definition 4.1.1. Take a Zero-Range process with $L+1$ sites labeled $(0, 1, ..., L)$. The rate $u_{i,j}$ from site i to site j is defined via

$$u_{ij} = \begin{cases} \mathbb{1}(\eta_i) & \text{if } i \neq 0 \\ c\mathbb{1}(\eta_i) & \text{if } i = 0 \end{cases}$$

where $0 < c < 1$.

4.2. Equilibrium

As in example 3.2.5 these rates can be written down as

$$c(\eta, \eta^{i,j}) = W_{i,j} u_i(\eta_i) \tag{4.1}$$

where

$$W_{i,j} = \frac{1}{L} \text{ for all } i, j \epsilon \{0, 1, 2, ..., L\} \text{ and } i \neq j \tag{4.2}$$

$$W_{i,i} = 0 \text{ for all } i \epsilon \{0, 1, 2, ..., L\} \tag{4.3}$$

and the total rates

$$u_i = \begin{cases} L * \mathbb{1}(\eta_i) & \text{if } i \neq 0 \\ L * c\mathbb{1}(\eta_i) & \text{if } i = 0 \end{cases}$$

4.3. Annihilation on a single slow site

In this section the dynamic situation of the single slow site system with an annihilation therm will be discussed. Because of the annihilation the equilibrium distribution will always be that there are no particles left. Therefore in order to know something about the system we need to start in a specific distribution η.

First the system with an annihilation therm is defined. For this thesis the annihilation probability is equal for all particles and times. This speed will be called α.

The generator $\mathcal{L}$ corresponding to such as system will be over a state space $\Omega = \mathbb{N}_0^{L+1}$, for arbitrary functions $f : \Omega \longrightarrow \mathbb{R}$ we get:

$$\mathcal{L}f(\eta) = \sum_{x=1}^{L}\sum_{y=0}^{L} \mathbb{1}_{\eta_x>0}[f(\eta-\delta_x+\delta_y)-f(\eta)]+c\sum_{y=1}^{L} \mathbb{1}_{\eta_0>0}[f(\eta-\delta_0+\delta_y)-f(\eta)]+\alpha\sum_{x=0}^{L} \eta_x[f(\eta-\delta_x)-f(\eta)] \tag{4.4}$$

Now we want to find what happens to the number of particles in the slow site and the non slow sites in this system.

Theorem 4.3.1. *For the zero range process with $\eta \in \Omega$ defined via the generator $\mathcal{L}$ in equation 4.4 for the functions $G_L(\eta(t)) = \frac{\sum_{x=1}^{L}\eta_x(t)}{L}$ and $H_L(\eta(t)) = \frac{\eta_0(t)}{L}$ when $L \longrightarrow \infty$ the pair $(G_L(\eta(t)), H_L(\eta(t))) \longrightarrow (g(t), H(t))$ where $g(t)$ and $h(t)$ are deterministic and satisfy the differential equations:*

$$\frac{d}{dt}g(t) = -\frac{g(t)}{1+g(t)} + c\mathbb{1}_{h(t)>0} - \alpha g(t) \tag{4.5}$$

$$\frac{d}{dt}h(t) = \frac{g(t)}{1+g(t)} - c\mathbb{1}_{h(t)>0} - \alpha h(t) \tag{4.6}$$

Proof. In order to show $(G_L, H_L) \longrightarrow (g, h)$ we need to show $\mathbb{E}(G_L) \longrightarrow g$, $\mathbb{E}(H_L) \longrightarrow h$ and that $\text{Var}(G_L) \longrightarrow 0$, $\text{Var}(H_L) \longrightarrow 0$. This proof is in 3 parts, first we show the expectation value is good.
Than we determine for a general Markov process a relation for the variance of any function. Than we use this to show that this variance of $G_L$and H_L go to zero when the system size increases.

First we want to show $\mathbb{E}(G_L) \longrightarrow g$, $\mathbb{E}(H_L) \longrightarrow h$
We calculate the effect of the generator 4.4 on the functions G_L and H_L.

$$\mathcal{L}G_L(\eta) = \sum_{x=1}^{L}[\mathbb{1}_{\eta_x>0}\frac{-1}{L}] + c\mathbb{I}_{\eta_0>0}\frac{1}{L}L + \alpha\sum_{x=1}^{L}[\eta_x\frac{-1}{L}] = -\frac{1}{L}\#_{>0}(\eta) + c\mathbb{1}_{\eta_0>0} - \alpha G_L(\eta) \tag{4.7}$$

and similar

$$\mathcal{L}H_L(\eta) = \frac{1}{L}\#_{>0}(\eta) - c\mathbb{1}_{\eta_0>0} - \alpha H_L(\eta) \tag{4.8}$$

where $\#_{>0} : \Omega \longrightarrow \mathbb{R}$ is the number of bulk sites with at least one particle. Thus $\#_{>0}(\eta) = \sum_{x=1}^{L} 1(\eta_x > 0)$

For a Markov process represented by the generator $\mathcal{L}$ and $\forall f : \Omega \longrightarrow \mathbb{R}$.

$$\frac{d}{dt}\mathbb{E}[f(\eta(t))] = \mathbb{E}[\mathcal{L}f(\eta(t))] \tag{4.9}$$

Make $g_L(t) := \eta_0[G(\eta(t))]$ and $h_L(t) := \mathbb{E}_{\eta_0}[H(\eta(t))]$ Now using equations (4.7).

$$\frac{d}{dt}g_L(t) = \mathbb{E}_{\eta_0}[LG(\eta(t))] = -\frac{1}{L}\mathbb{E}_{\eta_0}[\#_{>0}] + c\mathbb{E}_{\eta_0}[\mathbb{1}_{\eta_0>0}] - \alpha g_L(t) \tag{4.10}$$

$$\frac{d}{dt}h_L(t) = \mathbb{E}_{\eta_0}[LH(\eta(t))] = \frac{1}{L}\mathbb{E}_{\eta_0}[\#_{>0}] - c\mathbb{E}_{\eta_0}[\mathbb{1}_{\eta_0>0}] - \alpha h_L(t) \tag{4.11}$$

One can show that as $L \longrightarrow \infty$ that

$$\frac{\mathbb{E}[\#_{>0}(\eta(t))]}{L} = \Phi(g(t)) \tag{4.12}$$

Where Φ can be approximated using the equilibrium distribution for the non slow sites without the annihilation, as the rate from one site to any other is large compared to the annihilation rate as $L \longrightarrow \infty$.

In section 3.2 we can see that for a transition rates $\propto \mathbb{1}(\eta_i > 0)$ we can see that the grand canonical reversible product measures are a geometric distribution for the product measure:

$$\mu_i(n) = \lambda^n(1-\lambda) \tag{4.13}$$

and for a lot of these states the average number of particles in those states.

$$\rho = \mathbb{E}_{\mu_i(n)}[n] = \sum_0^\infty \lambda^n(1-\lambda) = \frac{\lambda}{1-\lambda} \tag{4.14}$$

where λ is the part of the sites with at least one particle, and thus we can write

$$\lambda = \frac{\rho}{1+\rho} \tag{4.15}$$

Using the replacement lemma in [4] we can use this to fill int $\Phi(\rho) = \frac{\rho}{1+\rho}$.

If we now Implement this in equations 4.10 and 4.11 as we take the functions g, h where $g(t) = \lim_{L\to\infty} g_L(t)$ and $h(t) = \lim_{L\to\infty} h_L(t)$

$$\frac{d}{dt}g(t) = -\frac{g(t)}{1+g(t)} + c\mathbb{1}_{h(t)>0} - \alpha g(t) \tag{4.16}$$

$$\frac{d}{dt}h(t) = \frac{g(t)}{1+g(t)} - c\mathbb{1}_{h(t)>0} - \alpha h(t) \tag{4.17}$$

This is a description for the limit large number of sites of the expectation, however in order to get convergence the variance should also go to zero when the system gets large.

First we want to show that for a Markov process $(\eta(t), t \geq 0)$ with rates $c(\eta, \xi)$ and generator $\mathcal{L}f(\eta)$ and a function from that statespace f the Dynkin-Martingale

$$M_t^f = f(\eta(t)) - f(\eta(0)) - \int_0^t Lf(\eta(s))ds \tag{4.18}$$

we want to show that $\mathbb{E}[M_t^f] = 0$, as $M_0^f = 0$ we can see that

$$\mathbb{E}[M_t^f | \eta(r), 0 \leq r \leq s] = M_s^t, \;\; 0 \leq s \leq t \tag{4.19}$$

with $s = 0$ has the same result, but this equivalent to

$$\mathbb{E}[M_t^f - M_s^f | \mathcal{F}_s] = 0, \;\; > s \tag{4.20}$$

we start with

$$\begin{aligned}\mathbb{E}[M_t^f - M_s^f | \mathcal{F}_s] &= \mathbb{E}[f(\eta(t) - f(\eta(s) - \int_s^t \mathcal{L}f(\eta(r)dr | \mathcal{F}_s] \\ &= S_{t-s}f(\eta(s)) - f(\eta(s)) - \int_s^t S_{r-s}\mathcal{L}f(\eta(s))\end{aligned} \tag{4.21}$$

Here we use that

$$\begin{aligned}\mathbb{E}(f(\eta(t))|\mathcal{F}_s) &= \mathbb{E}(f(\eta(t))|\eta_s) \\ &= \mathbb{E}_{\eta_s}(f(\eta(t-s))) \\ &= S_{t-s}f(\eta(s))\end{aligned} \tag{4.22}$$

We also have that

$$S_{r-s}\mathcal{L}f(\eta(s)) = \frac{d}{dr}S_{r-s}f(\eta(s)) \tag{4.23}$$

Therefore we fill that into the integral

$$\mathbb{E}[M_t^f - M_s^f|\mathcal{F}_s] = S_{t-s}f(\eta(s)) - f(\eta(s)) - (S_{t-s}f(\eta(s)) - f(\eta(s))) = 0 \tag{4.24}$$

and we have shown that M_t^f has expectation value 0 for all t and therefore is a Martingale.
Now we define $[M_t, M_t]$ as the unique increasing process such that

$$M_t^2 - [M_t, M_t] = \tilde{M}_t \tag{4.25}$$

where $\tilde{M}_t$ is a martingale.

This results in

$$\mathrm{Var}(M_t) = \mathbb{E}[M_t^2] = \mathbb{E}([M_t, M_t]) \tag{4.26}$$

the quadratic variation of martingale M_t^f can be computed as follows

$$[M_t^f, M_t^f] = \int_0^t \Gamma(f)[\eta_s]ds \tag{4.27}$$

where

$$\Gamma(f) = \mathcal{L}f^2 - 2f\mathcal{L}f = \sum_{\xi}(f(\eta) - f(\xi))^2 c(\eta, \xi) \tag{4.28}$$

Now one can fill in for f_L both G_L and H_L, and prove $M_t^{G_L}, M_t^{H_L} \longrightarrow 0$

For G_L we get

$$\Gamma(G_L) = \sum_{\eta'} c(\eta, \eta')\frac{1}{L^2}\sum_{x=1}^{L}[\eta_x - \eta'_x] \leq \sum_{\eta'}\frac{2}{L^2} = \mathcal{O}(\frac{1}{L}) \tag{4.29}$$

Where we use that there are only 2 sites x where $\eta_x \neq \eta'_x$ and $c \neq 0$. Also $c(\eta, \eta') \leq 1$.

This means that for $L \longrightarrow \infty$, $\mathrm{Var}(G_L(t)) \longrightarrow 0$. And therefore $G_L \longrightarrow g(t)$.

Now for H_L we have

$$\Gamma(G_L) = \sum_{\eta'} c(\eta, \eta')[H(\eta) - H(\eta')]^2 = \sum_{\eta'} c(\eta, \eta')\frac{1}{L^2}[\eta_0 - \eta'_0]^2 = \mathcal{O}(\frac{1}{L}) \tag{4.30}$$

This means that for $L \longrightarrow \infty$, $\mathrm{Var}(H_L(t)) \longrightarrow 0$. And therefore $H_L \longrightarrow h(t)$. □

5

Relation between zero range processes and statistical physics

In this chapter some parts of statistical physics is explained and connected to the mathematical models of previous chapters.

5.1. Counting states for different types of particles

In statistical physics, the number of quantum states a single particle can be in is countable. We presume they are finite now. In this thesis we will call a quantum state of a single particle a spin-orbital. This means quantum mechanically indistinguishable including spin degeneracy. Initially we presume all spin-orbitals have equal energy. In section 5.3 we will show what happens when the energy is not the same.

When multiple particles that do not interact with one another, and have the same forces act upon them, we can consider the combined state. The combined state of multiple particles is a linear combination of product of single particle states.
For fermions we have that there is no possible way to combine the single particle wave becouse of their asymmetric wave function. This means fermions can never be in the same state as another identical fermion.
For identical bosons the wave function is symmetrical and this makes that the wave function to be the same under exchange of particles in states, and therefore the combined state of multiple particles has no multiplicity. We will not go into the quantum mechanics but just use these results.

5.1.1. Classic particles

Classic particles are particles that are distinguishable from one another. Therefore if we have the state of each particle as a random variable (equal to probability for set particle to be at a certain site), the combined probability distribution is the multiplication of the random variables.

Example 5.1.1. *Take 2 particles and two sites they can be at. (in physics these sites are unique quantum mechanic solutions).*
-classic particles: If the particles are classic particles i.e. they can be distinguished from one another. There are 2^2 *possible states the system can be in.*

5.1.2. Fermions

Fermions are particles that have odd eigenfunctions of the Schrödinger equation. As a result of this they do not have a quantum solution with 2 of the exact same spin-orbital. In practice this means there is no way 2 fermions are in the exact same quantum state and therefore not in the same spin-orbital.

Example 5.1.2. *If we have 2 fermions that can occupy two orbitals, when these orbits are quantum mechanical identical for both particles there is only one way these particles can distribute, one in each*

spin-orbital.

5.1.3. Bosons

Bosons, like fermions are indistinguishable particles. Therefore one cannot simply multiply the individual probability densities. There is no difference between the order of the particles as they all are equal. Therefore when we describe a state of the system it is a combination of each orbital and how many particles are in that orbital. This also corresponds to all states of the system possible.

Example 5.1.3. *If we take two Bosons that can occupy any combination of two sites (quantum states of the single particle) there are 3 ways that the particles can be distributed:*
- two particles at site A
- two particles at site B
- one particles at site A and one at site B
It turns out that when there is no interaction between the particles and the sites are distinguishable, but otherwise equal the probability for the location of the particles is uniform and therefore in this example when we look at the state of the system there is a 1/3 chance to find the system in one of the states enumerated above.

When we assume all states have the same energy in theory all possible states of the system have the same probability in equilibrium. However different particle types have different states that are valid as discussed above. Therefore the equilibrium probability distribution is constant for all states.

We can take the set of these states as Ω for a zero range process and in order to model particle movement design Zero range processes such that their detailed balance is equal to the equilibrium of a system of particles in quantum states.

5.1.4. Equilibrium positions for different particle types

To make the different particle types even more clear we will calculate the equilibrium probability distribution for N particles that can be at L different sites in case the particles behave classical, fermion like or boson like.

Classical particles
The number of (micro)states is L^N every particle has L places it can be. Every combination is valid as the particles are distinguishable.

Fermions
The number of (micro) states for fermions is $\binom{L}{N}$ since there can be only one particle per site it is any group of size N out of L possibilities. Note that the number of sites must be larger than the number of particles.

Bosons
Now for bosons it is $\binom{N+L-1}{N}$. In order to see this think of a line of N+L-1 sites and pick L-1 of them random. The ones picked indicate a next orbital, the length of connected not chosen sites is the number of particles at that site. This is a bijection between the set of states and $L-1$ choices out of a set of $N+L-1$ and therefore the number of possible distributions of N bosons over L sites is $\binom{N+L-1}{L-1} = \binom{N+L-1}{N}$.

5.2. Equal rates and counting states

5.2.1. Classic particles

In the previous section the states are counted. In this section we will show how we can make a zero range process with the same probability distribution.

Presume all rates of a system of a set number of particles N in set number of sites L is the same for all sites. Take this rate $c(\eta, \eta^{i,j}) = c * \eta_i$ now we calculate the equilibrium position.

$$\nu_{L,N}(\eta) = \frac{\prod_{i=0}^{L-1} \frac{1}{\prod_{j=1}^{\eta_i} c*\eta_j}}{Z_{L,N}} = \frac{\frac{1}{\eta_i!}}{\sum_{\eta':\sum_{i=0}^{L-1}\eta'_i=N} \frac{1}{\eta'_i!}} \tag{5.1}$$

Now we calculate Δ the number of ways one can have N unique particles distributed as η over L sites.

$$\Delta_\eta = \frac{N!}{\prod_{i=0}^{L-1} \eta_i} \tag{5.2}$$

If now we want to know the equilibrium distribution of N independent walks over length L we have to normalize Δ

$$\frac{\Delta_\eta}{\sum_{\eta':\sum_{i=0}^{L-1}\eta'_i=N} \Delta'_\eta} = \frac{\frac{1}{\eta_i!}}{\sum_{\eta':\sum_{i=0}^{L-1}\eta'_i=N} \frac{1}{\eta'_i!}} \tag{5.3}$$

And thus Δ_η and $\nu_{L,N}(\eta)$ have the same equilibrium distribution.

5.2.2. Bosons

Now when we take a system where $c(\eta, \eta^{i,j}) = c * \mathbb{1}(\eta_i)$

$$\nu_{L,N}(\eta) = \frac{\prod_{i=0}^{L-1} \frac{1}{\prod_{j=1}^{\eta_i} c}}{Z_{L,N}} = \frac{\frac{1}{N}}{\sum_{\eta':\sum_{i=0}^{L-1}\eta'_i=N} \frac{1}{N}} \tag{5.4}$$

and we get the result that all distributions of particles are equally likely in equilibrium, this is the boson behaviour from the previous section.

But we can describe more zero range processes such that they have the same distribution as a boson gas with all states equally likely. If we have all states equally likely and we have detailed balance it must be true that

$$c(\eta, \eta^{i,j}) = c(\eta^{i,j}, \eta) \tag{5.5}$$

But this can change for any pair i, j. We can make a symmetric matrix C of size $L \times L$ where

$$C_{i,j} \mathbb{1}_{\eta_i > 0}(\eta_i) = c(\eta, \eta_{i,j}) \tag{5.6}$$

Here the symmetry of the matrix guarantees symmetry in the rates, $c(\eta, \eta_{i,j}) = c(\eta_{i,j}, \eta)$. This is because the indication function is symmetric for $\eta_i \neq 0$ and $\eta_j^{i,j} \neq 0$. If $\eta_i = 0$ we get $\eta_i^{i,j} = -1$ and this is not a valid state. $\eta_j^{i,j}$ cannot be zero as it is the state where we have one particle hop from i to j.

In summary, for two states η, ξ in a zero range system, if there are $i, j \leq L$ such that $\xi = \eta^i, j$ than we have $c(\eta, \xi) = c(\xi, \eta) = C_{i,j}$ and if there are not such $i, j \leq L$ we have $c(\eta, \xi) = c(\xi, \eta) = 0$. This results in an equilibrium position where all states of the system are equally likely.

5.3. Probability and energy

In statistical physics, however, the equilibrium distribution is influenced by the energy of that state. In this thesis we will presume every particle has an energy corresponding to the site it belongs to. The total energy E of a state η is the sum of the energy E_i of each site i times the number of particles in set site η_i.

$$E(\eta) = \sum_{i=0}^{L-1} E_i * \eta_i \tag{5.7}$$

Now for the equilibrium distribution μ depends on the temperature according to

$$\mu(\eta) \propto e^{-\frac{E(\eta)}{k_b T}} \tag{5.8}$$

where T is the temperature in Kelvin, and k_b is the Boltzmann constant. This needs to be normalized so that $\sum_{\eta\in\Omega} \mu(\eta) = 1$.

Thus comparing the equilibrium probability density μ of a state $\hat{\eta}$ with energy $\hat{E}$, and state $\check{\eta}$ with energy $\check{E}$ we know

$$\frac{\mu(\hat{\eta})}{\mu(\check{\eta})} = e^{\frac{\check{E}-\hat{E}}{k_b T}} \tag{5.9}$$

If we now take some η such that $\eta_i \neq 0$ and $\eta^{i,j}$ ($\eta_j^{i,j} \neq 0$ is guaranteed as $\eta_j^{i,j} = 0 \implies \eta_j = -1$ is not possible). Take the energy of these sites as defined in 5.7. Now $E(\eta) = \sum_i \eta_i * E_i$ and $E(\eta^{i,j}) = \sum_i \eta_i^{i,j} * E_i$.

$$\frac{\mu(\eta)}{\mu(\eta^{i,j})} = e^{\frac{\sum(\eta_i - \eta_i^{i,j})E_i}{k_b T}} = e^{\frac{E_i - E_j}{k_b T}} \tag{5.10}$$

Take rates such that

$$c(\eta, \eta^{i,j}) = c(\eta^{i,j}, \eta) e^{\frac{E_i - E_j}{k_b T}} \tag{5.11}$$

and the system will be in equilibrium for bosons with the energy of the states as prescribed.

A more explicit method to express the rates is obtained using the matrix C as in equation 5.6. Now the rates

$$c(\eta, \eta^{i,j}) = C_{i,j} e^{\frac{E_i - E_j}{2k_b T}} \tag{5.12}$$

satisfies equation 5.10 and therefore is in detailed balance for μ that satisfies equation 5.8.

Example 5.3.1. *Lets take a 2 particle 2 site system but now for $E_2 - E_1 = k_b T$. Now we calculate the equilibrium distribution. Notate $[2, 0]$ the state where there are 2 particles in state 1 and 0 particles in state 2.*

$$\mu([2,0]) = \mu([1,1])e^{-1} = \mu([0,2])e^{-2} \tag{5.13}$$

As these are all possible states and we get the canonical ensemble

$$Z_{2,2} = 1 + e^{-1} + e^{-2} \tag{5.14}$$

and we get

$$\begin{aligned} \mu([2,0]) &= \frac{1}{1 + e^{-1} + e^{-2}} \\ \mu([1,1]) &= \frac{e^{-1}}{1 + e^{-1} + e^{-2}} \\ \mu([0,2]) &= \frac{e^{-2}}{1 + e^{-1} + e^{-2}} \end{aligned} \tag{5.15}$$

5.4. Bose-Einstein condensation

5.4.1. States of matter

Bose Einstein condensate is a state of matter. The most commonly known states of matter are solid, liquid and gas. In solids particles have a set place, in liquids particles can move, but the particles stay together and therefore occupy a non variable volume. gasses have particles that are free to move apart from one another.

However in solids, fluids and gasses particles have a distinct place, and therefore behave as classical particles. In all these cases an increase in particles means that in constant volume the pressure increases and at constant pressure the volume increases.

When the matter becomes a Bose Einstein condensate the maximum pressure of the system is reached and adding more particles in the same volume will not increase pressure.

In statistical physics we have a chemical potential $\hat{\mu}$ that has a relation to the expected number of particles at a site. In this thesis we use $\hat{\mu}$ for the chemical potential to prevent confusion with μ the probability density function.
For bosons the expected number of particles at a site is given by the Bose Einstein distribution as we will show in 5.4.2

$$\hat{N}(E_i) = \frac{1}{e^{\frac{E_i - \hat{\mu}}{k_b T}} - 1} \tag{5.16}$$

When the chemical potential goes to the the energy of the state the number of particles in that state goes to infinity.

This asymptotic behaviour makes it problematic that when the chemical potential $\hat{\mu} \longrightarrow E_0$ where $E_0 = \min(E_i)$, the total number of particles in the system is limited. At this point the equivalence of ensembles holds no more. For the particles added the entropy of being in a higher energy state is equal to the increase in energy to get to these states at that temperature. Therefore the likelihood of being in these higher energy states does not increase while the density of particles does increase.

For classical particles this does not happen because they all have independent multiplicity. Fermions simply cannot be at the same site. Therefore this can only happen with bosons.

5.4.2. Bose Einstein distribution

For systems where the energies are distributed as in section 5.3 the grand canonical ensemble becomes [5].

$$\mathcal{Z} = \prod_{j=\text{site}} \sum_{n_j=0}^{\infty} e^{\beta(\hat{\mu} - E_j)n_j} \tag{5.17}$$

This leads to a converging probability distribution when the chemical potential $\hat{\mu} \leq E_i$ for all sites i. This probability distribution is known as the Bose Einstein distribution

$$\overline{n_i} = \frac{1}{e^{\beta(E_i - \hat{\mu})} - 1} \tag{5.18}$$

5.4.3. Infinite BEC

In section 9.3 in[**StatPhys**] it is shown that a 3D ideal Bose gas that is dense enough at a certain fixed temperature T creates a Bose Einstein condensate. For such a system the energy of a free particle is $E_{\text{kin}} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$, and we get

$$N = \sum_k \frac{1}{e^{\beta(\frac{\hbar^2 k^2}{2m} - \hat{\mu})} - 1} \simeq \frac{V}{(2\pi)^3} \int_0^\infty \frac{1}{e^{\beta(\frac{\hbar^2 k^2}{2m} - \hat{\mu})} - 1} 4\pi k^2 dk, \tag{5.19}$$

where N is the total number of particles and $\beta = \frac{1}{k_b T}$, k_b the Boltzmann constant and T the absolute temperature.

This integral can be rewritten so that we get

$$\frac{N}{V} = \frac{4(2m\pi k_b T)^{\frac{3}{2}}}{\sqrt{\pi}\, h^3} \int_0^\infty \frac{x^2}{e^{x^2 - \beta\hat{\mu}} - 1} dx \tag{5.20}$$

This integral is finite, and when $\beta\hat{\mu} \longrightarrow 0$ we have $\frac{4}{\sqrt{\pi}} \int_0^\infty \frac{x^2}{e^{x^2 - \beta\hat{\mu}} - 1} dx \simeq 2.61$.

This means there is only a set number of particles that can be in this distribution. However there is no such limitation on the physical system, as any orbital has no limit on the number of particles.

What will happen is that the chemical potential reaches the lowest energy orbital as the number of particles increases. Here the $\simeq$ symbol in equation 5.19 will not be valid and the first term of this sum must be taken separately. As $\hat{\mu} \longrightarrow 0$ we have $n_0 \longrightarrow \infty$. For all other orbitals the chemical potential stays the same and occupation of those orbitals does not change and we get

$$N = N_0 + \frac{4(2mk_bT)^{\frac{3}{2}}}{\sqrt{\pi}h^3} V \int_0^\infty \frac{x^2}{e^{x^2}-1} dx \tag{5.21}$$

The result is a system with 2 regimes. If the particle density is low enough all orbitals get extra particles. As the particle density increases then at some density all particles added by increasing the density go to the orbit with the lowest energy. The state where all particles go to the lowest energy site is known as a Bose-Einstein condensate.

This also happens for other systems. We will explore the case of harmonic oscillators in 1D and 3D. To do this we use we use that the total number of particles

$$N = \int_0^\infty \frac{g(E)}{e^{\beta(E-\hat{\mu})}-1} dE \tag{5.22}$$

where $g(E)$ is the density of states over energy for particles. For any systems, if we change all the energies of the orbitals by the same amount, and change the chemical potential by the same amount we will have the exact same system. Therefore we can make the systems such that the lowest energy orbital has energy 0. Therefore we also have $\hat{\mu} \leq 0$.

Example 5.4.1 (1D harmonic oscillator)**.** *We have an oscillator that has energy levels* $[\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, ..., \infty]$. *But we can compensate all with* $-\frac{1}{2}\hbar\omega$ *and we have energy levels* $[0, 1, 2, ..., \infty] * \hbar\omega$.

Unlike the free boson gas this does not have a set volume V*, however we can make the system larger by taking a wider potential energy function because a wider potential energy function, i.e. the spatial distribution becomes larger, creates higher density spacing of energy levels. So we have a set density* $\rho = N * \hbar\omega$.

For this system when $N \longrightarrow \infty$ *we have* $g(E) = \frac{1}{\hbar\omega}$ *therefore.*

$$N = \frac{1}{\hbar\omega} \int_0^\infty \frac{1}{e^{\beta(E-\hat{\mu})}-1} dE \tag{5.23}$$

However this integral does not converge. As explained in [3] for finite numbers of bosons particles a transition to the BEC phase occurs. It is well known that the thermodynamic limit predicts that a Bose Einstein Condensate is not possible for this 1D harmonic oscillator system.

Example 5.4.2. *Now the sites correspond to those of a 3D harmonic potential, thus we have the same energy levels as 5.4.1 but now the levels have multiplicity* $\frac{(n+1)(n+2)}{2}$ *for energy* $E_n = n\hbar\omega$. *Also the volume is 3 dimensional thus we get* $\rho = N(\hbar\omega)^3$.

Now we have

$$[3Dharmonicoscillator]g(E) = \frac{(\frac{E}{\hbar\omega}+1)(\frac{E}{\hbar\omega}+2)}{2\hbar\omega} \tag{5.24}$$

note here that this is the density of states, as we have that there is an energy level every $\hbar\omega$ *this is compensated for in the denominator.*

Now as we have the limit $\hbar\omega \longrightarrow 0$ *we get* $g(E) \longrightarrow \frac{E^2}{2(\hbar\omega)^3}$ *and therefore*

$$N = \frac{1}{2(\hbar\omega)^3} \int_0^\infty \frac{E^2}{e^{\beta(E-\hat{\mu})}-1} dE = \frac{(k_bT)^3}{2(\hbar\omega)^3} \int_0^\infty \frac{x^2}{e^{x-\beta\mu}-1} dx \simeq \frac{(k_bT)^3}{2(\hbar\omega)^3} * 2.404 \tag{5.25}$$

Now at a certain temperature the density in the system is finite. This is when $\rho = 1,202(k_bT)^3$ [5]. If the density becomes any larger the excess particles all go to the ground level. For the infinite sized system this will mean that there is an infinite amount of particles in the state with the lowest energy.

In a more general sense for systems of infinite size we can determine a density of particles. We can compute the resulting chemical potential. If there is a point where the chemical potential has to become higher than the lowest energy state that is not possible as the equilibrium will always want to put more particles in that state.

Therefore we have a system where if $\rho \leq \rho_0$ for some ρ_0 such that $\hat{\mu} = \min_i\{E_i\}$, then we have for any orbital i with energy E_i, the expected number of particles in that site is given by equation 5.18, where $\hat{\mu}$ is such that the density of the system is correct. When $\rho > \rho_0$ we get in a new regime where the number of particles in the lowest energy becomes macroscopic. Here for the limit of large systems we have $N \longrightarrow \infty$, and $\frac{N_0}{N} > 0$ and thus $N_0 \longrightarrow \infty$ which means that $\hat{\mu} \longrightarrow E_0$ and thus that in the limit the chemical potential becomes equal to the lowest energy of sites. The expected number of particles in any orbital other than the lowest energy one will be determined with equation 5.18 again. For the lowest energy site infinitely many particles will be present. We can determine the part of the total particles by $1 - \frac{\rho_0}{\rho}$, as $\frac{\rho_0}{\rho}$ will be the fraction of particles in the non condensed states. This is because the Bose-Einstein distribution for $\hat{\mu} = \min_i\{E_i\}$ this will be the number of particles in the excited sites.

5.4.4. Finite BEC

In the previous subsection we presume the system size to be infinite. However in chapter 6 we do simulations and we can only do simulations on finite systems. Also a Bose Einstein condensate made out of particles that spontaneous disappear will probably be relatively small for a system. Therefore we explore how Bose-Einstein condensation changes when the system is not infinitely large.

For this section we will presume the system is large enough that the grand canonical ensemble is a good approximation [3]. However, the system is not so large that we can presume that the sum over all states becomes an integral over energy.

We take the sum of the expected number of particles over all sites with $x = e^{-\beta\hbar\omega}$ and the fugacity $z = e^{\beta\hat{\mu}}$ that is related to the chemical potential.

In [3] this procedure is used to compute the total number of particles in a 3D harmonic potential with energy levels $n\hbar\omega$ to be.

$$N = \sum_{j=1}^{\infty} \frac{z^j}{(1-x^j)^3} \tag{5.26}$$

Now one can numerically determine the fraction of particles at energy 0 from the number of particles and the temperature. In [3] this is done for $N = [100, 1000, 10000]$ and also computed analytically for the infinite system. In chapter 6 we will compare the $N = 100$ results from [3] to the results of the computations done in that chapter based on a Zero Range process.

5.5. Annihilating particles BEC

A condensate of particles that annihilate quickly, for example positronium atoms, is not realized in physical experiments yet. In this section we have seen that a zero range process has the same equilibrium distribution as the known systems, and can be used to get a theory about what happens if we have BEC with particles that annihilate. In section 5.3 we have seen that bosons in equilibrium have the same probability distribution as a zero range process with rates as in equation 5.12. In these models we can add an annihilation term like we did in chapter 4 for a system with a single slow site.

In this thesis we will not analytically compute the differential equations for these systems, as it is a more complicated than the single slow site problem. Therefore we will approximate these differential equations and then numerically calculate the results of those equations.

6

Simulations

In this chapter some simulations will be discussed. There are two concepts that are verified with these simulations. First we will do some realizations of the system in chapter 4. After that we will introduce an approximation of a zero range process designed to imitate a 3D harmonic oscillator in its equilibrium distribution. Then this model is compared to the results of [3]. Then we can take the same model but add an annihilation rate and see how this changes the system.

6.1. Single slow site simulation

In chapter 4 we computed the dynamics in the limit of large systems for a system with a single slow site and uniform transitions. In this section we will do a simulations of such systems, but finite in size. The simulations will be done for a range of system sizes so we should see the simulations will look more similar to the system the larger of a system we simulate.

The simulations are realizations of a stochastic system that has a state space that increases exponentially with system size, i.e. $\#\Omega = \mathcal{O}(e^L)$. Therefore it makes no sense to analyze every site combined. We can however compute the expected number of particles in the slow site and use statistics on that.

The goal of these simulations is to show how the simulations converge on the results of equations 4.16 and 4.17 when the system size increases.

6.1.1. Method

The simulations are done using python. The exact code can be found in the appendix A. This code is based on a code by Stefan Grosskinsky

We start with a range of number of sites of the set $[64, 128, 256, 512, 1024, 2048]$. For each of these the simulation is executed.

We create an array of length equal to the number of sites, where each element of the array correspond to the number of particles in that site. The time until the next jump is a random value, however the time it takes to have a certain number of jumps is Poisson distributed. In the simulations this is not taken into account. What we do compute is the total rate at which any hop or annihilation happens and take the time step.

Initial condition

This simulation is a random process. In this simulation the initial state is the equilibrium position of the system without annihilation. We need a realization of the equilibrium distribution as we need a specific state η for the system to be in.

We have for $L \longrightarrow \infty$ that the probability to have 0 particles in the slow site $P(\eta_0 = 0) \longrightarrow 0$. For detailed balance we need rate c from the slow site to any other site and rate 1 from any other site i to

the slow site that

$$c * P(\eta_0 \neq 0) = 1 * P(\eta_i \neq 0) \tag{6.1}$$

To compute the non-annihilation equilibrium for every non-slow site we take example 3.2.4 as this has the indication function for transition rates. So μ_i is a geometric distribution, and as $P(\eta_0 \neq 0) \longrightarrow 1$ we get $P(\eta_i \neq 0) = c$ we have a geometric distribution function with probability c to have at least one particle:

$$\text{for} \quad i \in \{1, ..., L\} \text{ we have} \quad P(\eta_i = n) = (1 - c)c^n \tag{6.2}$$

Now we simply take a realization of this probability distribution as our initial condition.

The slow site has condensation and therefore we cannot use the product measure as the number of particles at this site. We do know the total number of particles in the system, and the number of particles in all other sites.

$$\frac{\sum_{i=0}^{L-1} \eta_i}{L} = \rho \tag{6.3}$$

and therefore

$$\eta_0 = L * \rho - \sum_{i=1}^{L-1} \eta_i \tag{6.4}$$

Here it is important that the system forms a condensate for these values of ρ, c, and that we have the limit $L \longrightarrow \infty$. In this thesis we are only interested in cases where the initial condition has condensation, and we estimate the limit $L \longrightarrow \infty$ with these simulations.

A single iteration
Now we have an initial state of the system η, we are going to simulate how the state evolves at random in accordance to the transition and annihilation rates.

In this simulation we take uniform transition rates to hop out of every non-slow site to any other site to be 1, and the annihilation rate to be 0.5. However in the code we divide every rate by a factor L, and later re scale the time by a factor $1/L$ to end with the same system.

We define 'rate' as the sum of all transition rates and annihilation rates that are possible. Now we take a random number between 0 and 'rate'. If this is smaller than the sum over all transition rates we make a transition, if not we make an annihilation step.

For a transition step we take a random site to jump from. If this site happens not to have a particle in it we do nothing. If there is a particle at this site we check whether it is the slow site, if this is the case we need to compensate the transition rate from 1 to c and therefore we need to take a chance c for a random transition to happen. For any other site we simply take a random site to hop to.

If we have an annihilation step we have to randomly pick one particle where all particles are equal. Next we have a lower resulting annihilation rate as there is one less particle. To compensate for this the total rate needs to decrease by the rate of a particle to annihilate.

The simulation is executed for slow site rate $c = 0.5$, an initial density of particles $\rho = 5$ and the annihilation rate $a = 0.5$. We continue evolving η this way until there are no more particles in the system.

This system evolves over time, however we never specified time. We do have rates. All rates must be expressed over the same time unit. This is the time t we have in graph 6.1.

6.1.2. Results

We want to compare the results to the result of equation $g(t)$(corresponds to non-slow sites) and $h(t)$ (corresponds to the slow site), from equations 4.16 and 4.17. As no analytical solution to this set of differential equations is known we approximate the solution of this initial value ordinary partial differential equation with the python odeint function from the scripy.intergrate library.

We plot the graphs $g(t)$ and $h(t)$ in a plot with the number of particles in the slow site divided by L, $H^L(t) = \frac{\eta_0(t)}{L}$ and the number of particles in all other sites combined divided by L, $G^L(t) = \frac{\sum_{i=1}^{L} \eta_i(t)}{L}$ for $L \in [64, 128, 265, 512, 1024, 2048]$. This is shown in figure 6.1.

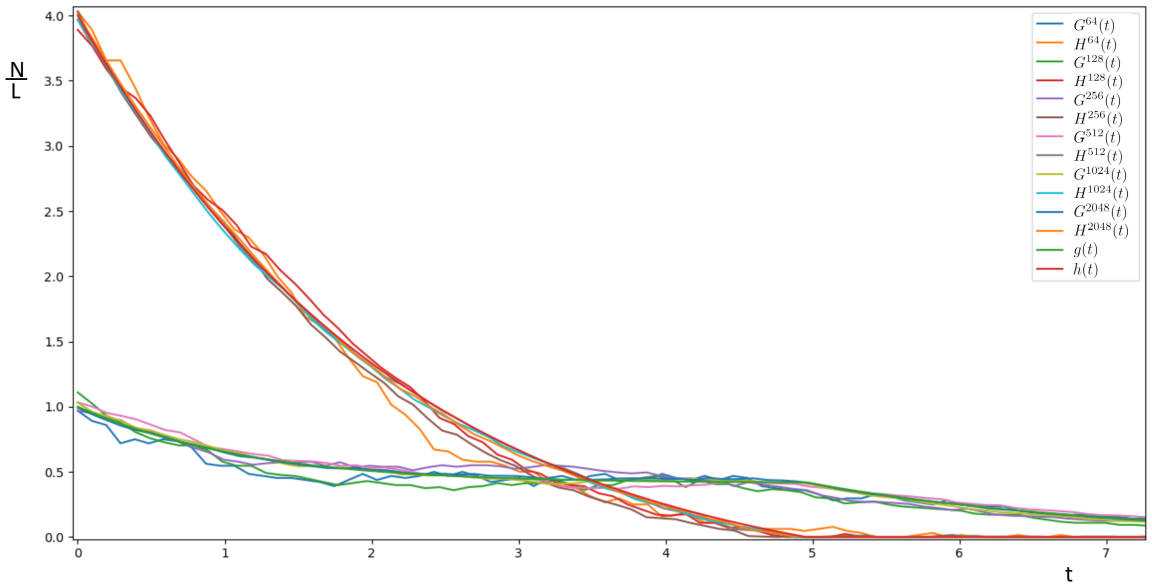


Figure 6.1: $G^L(t)$ and $H^L(t)$ realizations for $L \in [64, 128, 256, 512, 1024, 2048]$, together with $g(t)$ and $h(t)$, for a slow site system with uniform transition rate 1 exempt for the slow site rates 0.5 and an annihilation rate 0.5

This graph is a little cluttered, but we can see that both $G^L(t) \longrightarrow g(t)$ for $L \longrightarrow \infty$ and $H^L(t) \longrightarrow h(t)$ for $L \longrightarrow \infty$. We did prove this in chapter 4, but here we gain some intuition on how this happens.

It seems the function $g(t)$ goes to some form of equilibrium at 0.5 until the condensate ends. Then it becomes just an exponential decay. Intuitive this can be understood. The condensate guarantees that particles from the slow site keep going to the other sites as it will always have rate c from the slow site to any other site. The system will go to the equilibrium where the rates going in and out of a site are equal. When we introduce an annihilation term we add an outgoing therm for every site. This means the equilibrium changes.

Also $g(t) + h(t)$ must be exponential decay as it is the sum over all states divided by L as

$$\frac{d}{dt}(g(t)+h(t)) = -\frac{g(t)}{1+g(t)} + c\mathbb{1}_{h(t)>0} - \alpha g(t) + \frac{g(t)}{1+g(t)} - c\mathbb{1}_{h(t)>0} - \alpha h(t) = -\alpha(g(t)+h(t)) \quad (6.5)$$

We can check this for the simulations in figure 6.1 by adding up $G^L + H^L$ for all simulated L.
In figure 6.2 we see that in the log plot the number of particles behaves linear, thus the number of particles decays exponentially. When the number of particles left in the system becomes small, the variance increases.

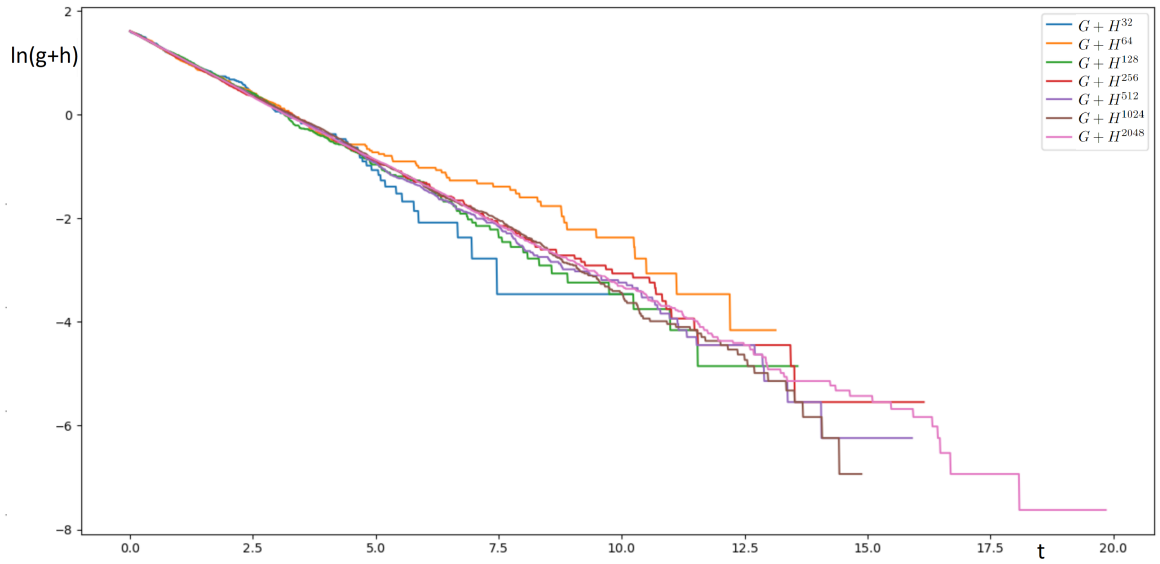


Figure 6.2: $Ln(G^L(t)+H^L(t))$ realizations for $L \in [32, 64, 128, 256, 512, 1024, 2048]$, for a slow site system with uniform transition rate 1 exempt for the slow site rates 0.5 and an annihilation rate 0.5

6.2. Annihilating bosons in 3-Dimensional harmonic potential

In this section we will not make a realization of the random process, but rather approximate the probability distribution for set times. Because $\#\Omega = \mathcal{O}(e^L)$ computing every state is too time intensive. Therefore we presume the probability distribution μ to be a product of the probability distribution μ_i of each site i. Each μ_i is a probability distribution that is a function of time.

In order to test if this is a reasonable assumption we can make the annihilation rate 0 and compare the equilibrium distribution to the results of [3].

6.2.1. Sites and their energy

First we need to set the energy of the sites the same as [3]. In order to do that we take

$$N = \sum_{j=1}^{\infty} \frac{z^j}{(1-x^j)^3} \tag{6.6}$$

where $x = e^{-\beta\hbar\omega}$, and $z = e^{\beta}\hat{\mu}$. Now for an i times excited state the energy of that state is $i\hbar\omega$. This state will have multiplicity $\frac{(i+1)(i+2)}{2}$.

We want to simulate a system that has infinite sites as it is a set of harmonic oscillator that has infinite eigenfunctions. The number of particles at those sites combined however is finite.

We can only simulate finite site systems, as the number of particles is finite there must be a finite set of sites that contain the vast majority of particles. The expected number of particles at a site at set temperature depends on the energy of that site. The higher the energy of the site the lower the number of particles in those sites. Therefore we take only m sites into account where according to the Bose Einstein distribution the probability to have 0 particles at that site is less than 99%. This is roughly equal to taking the expected number of particles in this site to be equal to 0.01.

We will use the same energy of states as in section 5.4.4. From here we can know $\beta\hbar\omega$. For the highest energy site m taken into account and P_m the expected number of particles at that site, $E_m = m\beta\hbar\omega$ is

the energy of the highest energy site. When $E_m\beta >> 0$, $\hat{\mu} \longrightarrow 0$ we get

$$P_m = \frac{1}{e^{E_m\beta} - 1} \simeq e^{-E_m\beta} \tag{6.7}$$

Which leads us to

$$m \simeq \frac{\ln(\frac{1}{P_m})}{\beta\hbar\omega} \tag{6.8}$$

and we pick m to be an integer such that the probability is about 0.01 to find a particle at a site with energy $m\hbar\omega$ at a certain temperature. Now m is the highest energy state number that we include in our computation.

6.2.2. Rates from energy

This simulation will be done using the transition rates explored in section 5.3. We take the elements $c_{i,j}$ of matrix C from equation 5.12 equal to $\frac{1}{(|i-j|)^3}$.

Because this simulation does not consider the general number of particles to be given, it results in states that are not possible. This effect can be compared to a grand canonical product measure that has nonzero entries for any number of particles. Only when we take the canonical ensemble these are multiplied by 0 for finite systems.

Because it is not possible to normalize the total distribution to the states that have N particles without a lot of computations, in this approximation the probability distribution of each site is computed. This approximation is similar to taking the grand canonical ensemble, we prescribe the total expected number of particles, but do not prohibit states that do not have the exact number of particles. With this approximation for every site we will end up with an equilibrium from the product measures. However in [3] the distribution of particles is presumed to follow the Bose-Einstein distribution, this by itself is a result of the grand canonical ensemble. In practice when we work with the expectation of the number of particles in the ground state this is not much of a problem as the probability for 0 particles to be in the ground orbit is small in both canonical and grand canonical ensemble.

This simplification does mean that the number of particles in states is not limited to the total number of particles set before, only their expectation. Therefore we have to consider $\mu_i(k) \neq 0$ for $k > N$. These μ_i have to be considered. The highest number of particles taken into account is $2N$. The probability to have more than $2N$ particles in one state according to the grand canonical ensemble must be insignificant for a system with 100 particles.

6.2.3. Differential equation

Now we have the rates, we can make the probability density functions change over time according to those rates, and therefore satisfy a set of differential equations. Every μ_i is $2N$ dimensional. Therefore on the matrix μ we can apply the Forward Euler method [2]. In order for the Forward Euler method to be stable we need an amplification factor that is sufficiently small.

$$\frac{d\mu_i^k}{dt} = -\sum_{j\neq i} c_{i,j}\mu_i^k \mathbb{1}(k>0) + \sum_{j\neq i} c_{i,j}\mu_i^{k+1} + \sum_{j\neq i}\sum_{l=1}^{2N} c_{j,i}\mu_j^l(\mu_i^{k-1} * \mathbb{1}(k>0) - \mu_i^k) \tag{6.9}$$

where μ_i^k is the probability to have k particles at site i. Now for stability it is not realistic to compute all eigenvalues of this problem but we can use that $d\mu_i^k << \mu_i^k$ for all i, k will probably be stable. We take $c_{i,j} = \frac{1}{L} - e^{\beta(E_i - E_j)}$ and we get

$$\sum_{j\neq i} c_{i,j} \leq e^m \leq 100 = \mathcal{O}(1) \tag{6.10}$$

and because every μ_i is a probability distribution

$$\sum_{l=1}^{2N} \mu_i^l \leq 1 \tag{6.11}$$

and thus we need $dt \leq \frac{1}{400}$. This is not a prove of stability, but rather an estimation for dt needed for stability.

6.2.4. Computation

The Python code is presented in appendix B. Here we will explain the steps taken.

We start from the initial condition with all 100 particles in the ground orbit. This means $\mu_{t=0}([100, 0, ..., 0]) = 1$.
First we establish a function called 'redis', this function has arguments: the matrix C, the energies E_i and the number of sites. It returns a matrix of transition rates, so $c_{i,j}$ as its entries.

Now we set the number of particles 'Np' to be 100. The temperature to be a range in terms of the condensation temperature of the infinite system to be an element of the array $[0.1, 0.2, ..., 1.2]$ using a for loop.

We compute from [3] that the energy density corrected for temperature, $\beta\hbar\omega$, in the code notated as 'bhw', to be

$$\beta\hbar\omega = \frac{1}{\frac{T}{T_c}N^{\frac{1}{3}} * g_3(1)} \tag{6.12}$$

we define the highest energy site m to be considered 'Nsmac' from the Bose-Einstein distribution. We presume condensation and therefore $\hat{\mu} \simeq 0$. Now for the i'th excited state we get the expected number of particles in that state:

$$\mathbb{E}(\mu_i(\beta\hbar\omega)) \simeq \frac{e^{-\beta i\hbar\omega}}{1 - e^{-\beta i\hbar\omega}} \tag{6.13}$$

Now for $\mathbb{E}(\mu_{i_{\text{max}}}) = 0.01$, we use 6.8 to compute 'Nsmac'. Now take $i_{\text{max}} = m$ the closest integer to $\frac{\ln(100)}{\beta\hbar\omega}$. This is how many energy levels we consider. The multiplicity of energy level $i = \frac{(i+1)(i+2)}{2}$. this needs to be taken into account.

Now for every site we first compute:

$$\sum_{j \neq i} c_{i,j} \tag{6.14}$$

and

$$\sum_{j \neq i} \sum_{l=1}^{2N} c_{j,i}\mu_j^l \tag{6.15}$$

because these are common factors in every difference equation. Than we change every μ_i^k with

$$\mu_i^k(t + \Delta t) = \mu_i^k(t) + \frac{d\mu_i^k(t)}{dt} * \Delta t \tag{6.16}$$

We repeat this for every site. Than we iterate 25000 times. We compute the average number of particles in the slow site $\mathcal{E}(\mu_0) = \sum_k \mu_0^k k$, divide that by the total number of particles and compare the resulting distribution to the graph in [3] figure 1. Here we see that the two graphs for 100 particles behave similar, However when $T \longrightarrow T_c$ we see the number of particles in the ground orbit becomes smaller than the results of [3]. This is because we do not change the chemical potential. This means the probability density function, we keep the same orbits and just increase the temperature.

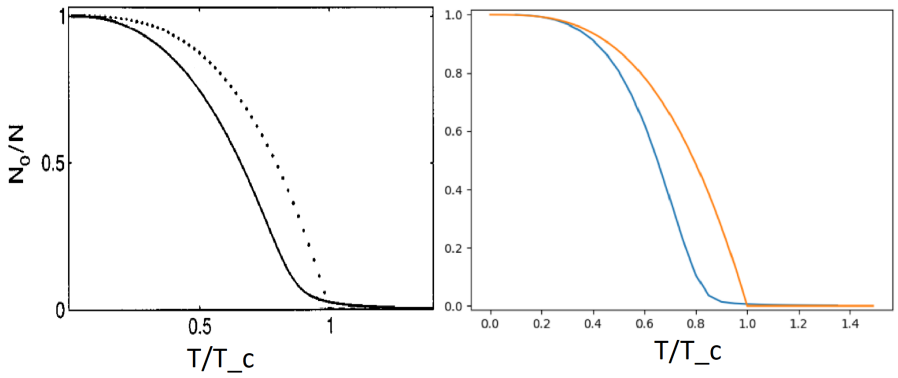


Figure 6.3: The number of particles in the ground state for a 100 particle 3D harmonic oscillator using [3] (left) and with the numerical approximation done in this thesis (right).

6.2.5. Annihilation

Now we have a model of this system, we can add an annihilation term to the numerical method. This factor will only apply to a single site probability density function μ_i which has elements μ_i^k where k is the number of particles in state i.

In this thesis we presume annihilation affects every particle individually. This means that annihilation rate $r \propto k$. This is problematic to model with forward Euler for high k. However if we have a certain probability distribution one can compute the probability distribution a certain time later using that the particles behave as independent particles.

The probability for one particle to annihilate is known, simply the annihilation rate r times the Δt (for small Δt). If we have k particles we have k independent variables all with probability $r\Delta t$ to annihilate from this we get a binomial distribution:

$$[\mu_i^l(t = t_0 + \Delta t)|\mu_i^k(t = t_0) = 1] = \binom{k}{l}(r\Delta t)^{k-l}(1 - r\Delta t)^l \tag{6.17}$$

This is from one specific occupation. However we can simply sum over the initial probabilities and we have the general case as this is a Markov process.

$$[\mu_i^l(t = t0 + \Delta t)|\mu_i(t = t_0)] = \sum_k \mu_i^k(t = t_0)\binom{k}{l}(r\Delta t)^{k-l}(1 - r\Delta t)^l \tag{6.18}$$

Implementation in code

Now we take the equilibrium of the 3D harmonic potential at temperature $\frac{T}{T_c} = 0.5$ as computed before. This will be the initial condition for the next simulation.

Now we keep evolving the same system but we take an annihilation rate in the series $[0.001, \frac{0.01}{3}, 0.01, \frac{0.1}{3}, 0.1, \frac{1}{3}, 1]$ times the redistribution rate of states with equal energy c. Now we plot the number of particles in the slow site vs the total number of particles in the system, as well as the number of particles in the first excited state vs the total number of particles.

For annihilation rates much slower than the redistribution rates $r << c$ the redistribution is done for so many times that the annihilation term is 0.03 times the redistribution rate. So for $r = 0.001c$ we do 30 re distributions without annihilation, than a annihilation step with 30 times the annihilation speed. This is done to reduce computations.

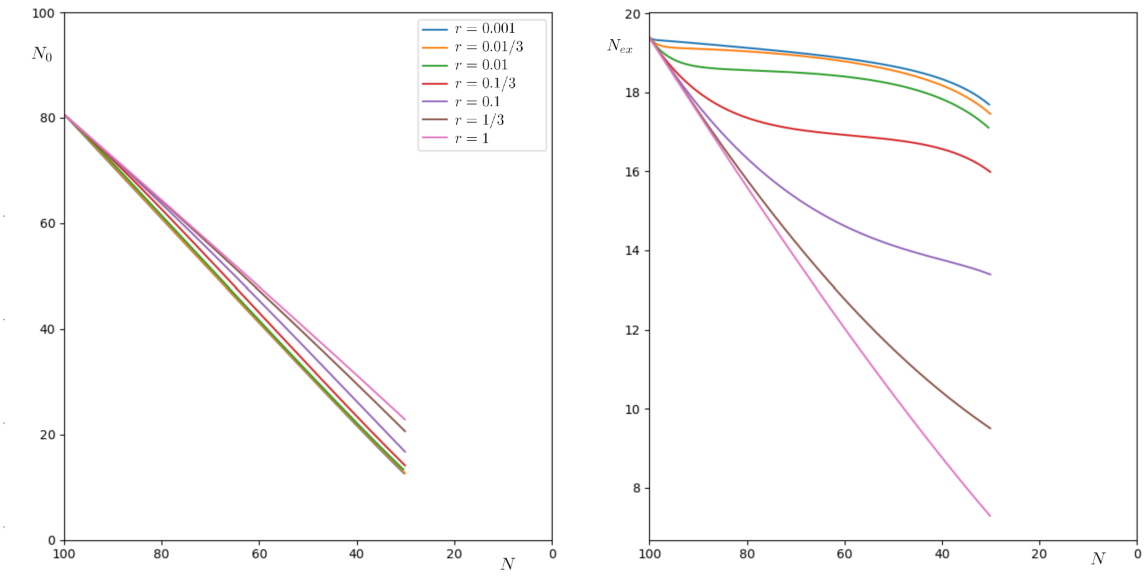


Figure 6.4: Number of particles in the ground state N_0 (left) and all excited states N_{ex} (right) for different annihilation rates all starting from the equilibrium of the system without annihilation and 100 particles at temperature $\frac{T}{T_c} = 0.5$

Note here that $N \propto e^{-\alpha t}$ we use N as the x-axis because this makes all graphs comparable. Because the annihilation rates differ a factor 10^3 and therefore a graph with time as the x-axis would not be use full.

On the right hand side of figure 6.4 we see that the slowest annihilation has the highest fraction of its particles in the excited states. This is because this system is closest to the equilibrium. As there is a condensate and we have fewer particles in the system they must come out of the ground orbit, since when we add them they would also go there.
The same can be observed in reverse in the number of particles in the ground state. The more time the system has to go to equilibrium means there are less particles left in the ground orbit.

Also like in section 6.1.2 the number of particles in the first excited site in figure 6.4(right) seems to stabilize as long as there is a condensate if we have a not too fast annihilation rate. As the annihilation rate increases the system has no time to form this semi equilibrium. At this point the annihilation is so much faster than the redistribution.

7

Discussion and conclusion

7.1. Conclusions

For a single slow site zero range process with uniform rates we have shown what the effect is of annihilating particles.

Also we have a working model of a 3 dimensional harmonic oscillator that reasonably behaves as the system described in [3]. However this is not exactly the same.

7.2. Discussion

7.2.1. Preservation of number of particles

In [3] it is presumed that the number of particles in the lowest energy state can be computed using the grand canonical ensemble and chose $\hat{\mu}$ so that the total number of particles is correct. However as we see in this thesis, for boson particles that are in a zero range process have a geometric distribution for the number of particles in the grand canonical ensemble. However when there is condensation probability distribution of particles at that site would behave like the canonical distribution and be more like normal distribution all round the expected number of particles, as it is equal to the total number of particles minus the number of particles in the other states that each on their own are geometrical distributed.

In this report we do not explore whether the model used for the 3D harmonic potential in this thesis behaves like the method in [3]. However the distribution for the condensed site had a probability distribution with a maximum probability close to the expected number of particles for the graphs used in this thesis. This distribution is not explored in this thesis, but can be done in future research.

It is possible that this because we started with all particles in the condensation site, and is not yet at the equilibrium of the differential equations in 6.2.3 but that this takes a longer time, and therefore the realizations are closer to the canonical ensemble. It makes sense that as the rates as a function of the number of particles in sites hardly change when the probability distribution of particles in the exited sites is correct, as the condensation site is almost in all distributions has at least one particle. Therefore the expectation of the number of particles in any sites does not change.

This effect however does not matter for annihilating particle systems as the particles in the system have annihilated before it can go to this geometric distribution.

7.2.2. Recommendations

A possible way to improve the approximation of the 3 dimensional harmonic oscillator is that the higher energy states are left out. But it is possible to make a term of classical behaving particles that also have interaction with the system. As all these sites have low occupation it is possible to model them

as classical particles. This would make it a lot less computationally intensive to estimate systems that are larger.

Also as discussed in the introduction in practice a BEC formed from positronium would probably be cooled using lasers. These lasers have an interaction with the positronium. We did not model anything like this.

In order to find out whether the assumptions done in this thesis about dense positronium cannot be verified as there is not yet an experiment where positronium is made dense and cold enough to be in a BEC. This means we can only see if this model is a good approximation when such an experiment is realized.

It might also be possible that annihilation's for bosons in a particular site would not increase when more than 1 particles is at this site, just like the transition rates. It is possible to implement this for the 3D harmonic oscillator computations in the future.

The system as simulated here requires there to be no interactions between particles. When one would need to take any interactions between particles in different sites it cannot be modeled as a Zero range process. For example a hard sphere interaction is not possible with a Zero range process as the rates between states would depend on the occupation of other states.

Bibliography

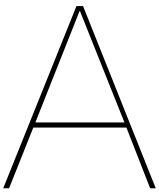
[1] M R Evans and T Hanney. “Nonequilibrium statistical mechanics of the zero-range process and related models”. In: *Journal of Physics A: Mathematical and General* 38.19 (Apr. 2005), R195–R240. DOI: 10.1088/0305-4470/38/19/r01. URL: https://doi.org/10.1088%2F0305-4470%2F38%2F19%2Fr01.

[2] M.B. van Gijzen. *Numerical methods for ordinary differential equations*. Delft Acedemic Press, 2015. ISBN: 9789065623737.

[3] Wolfgang Ketterle and N. J. van Druten. “Bose-Einstein condensation of a finite number of particles trapped in one or three dimensions”. In: *Phys. Rev. A* 54 (1 July 1996), pp. 656–660. DOI: 10.1103/PhysRevA.54.656. URL: https://link.aps.org/doi/10.1103/PhysRevA.54.656.

[4] C. Kipnis and C. Landim. *Scaling Limits of Interacting Particle Systems*. Grundlehren der mathematischen Wissenschaften. Springer Berlin Heidelberg, 1998. ISBN: 9783540649137. URL: https://books.google.nl/books?id=eLUNVIoYcOoC.

[5] Jos Thijssen. “Lecture notes Statistical Physics TN2624 - spring 2018”.



Python code used to simulate the single slow site system with annihilation

```
# Load some packages (if you get an error, you need to install the package in the terminal)
import numpy as np
import matplotlib.pyplot as plt
from scipy import linalg as lg
from scipy.stats import uniform
import time
from scipy.integrate import odeint
from cycler import cycler
monochrome = (cycler('color', ['k']) * cycler('marker',['', '.', 'o']))* cycler('linestyle',
', '--', ':', '-.'])
plt.rc('axes', prop_cycle = monochrome)
markn = 100
reps = 1

### Parameters ###

n = 8

Li=[32, 64, 128, 256]#, 512, 1024, 2048]    ## of sites
tau = []
slow = []
non_slow = []


c=0.5    #rate for slow site
rho = 5

for i in range(len(Li)):
    for r in range(reps):
        L = Li[i]

        lattice=np.arange(0,L)

        a=.5/L    #removal rate
        nn=rho*L     ##initial number of particles
        lc=L-1.+c/c     ##total

        rate=lc+a*nn     ##total jump rate
```

```
   N = nn+0        ## reset number of particles

   wait=1./rate   ##average waiting time
   deltat=L*N*wait/500

   conf=np.array([],dtype=int)    ##output list

   #######  Initialize  ##########

eta = np.random.geometric(p=c, size=L)-1   ##geometric initial condition
  total = np.sum(eta)                        ##number of bulk particles

if (total<nn):                    ##rest on condensate, condensed initial condition
       eta[0]+=(nn-total)
       N=nn

   else:
       N=total

conf=np.array([eta])           ##storing full particle configurations (not necessa

bulk=np.array([N-eta[0]])       ##number of bulk particles, condensate, and times
   cond=np.array([eta[0]])
   times=np.array([0])

   t=0.0
   nextout=deltat
   sample = 0

   while (N>0): # loop until done
       while (t<nextout and N>0):
 #          wait=np.random.exponential(meanwait) # random holding time

        if (uniform.rvs(0,rate) < lc):    ##jump dynamics, choose a site
                pos=np.random.randint(L)
  #                  ll=len(  [pos])
                if (eta[pos]>0):
                    if (pos==0):
                        if (uniform.rvs() < c):
                            eta[pos]-=1
                            pp=np.random.randint(1, L)
                            target=(pos+pp)%L
                            eta[target]+=1

                    else:
                        eta[pos]-=1
                        pp=np.random.randint(L)
                        target=(pos+pp)%L
                        eta[target]+=1

      else:                       ##evaporation dynamics, choose a particle
                pos=np.random.choice(lattice,1,p=(eta/N))
                eta[pos]-=1
                N-=1
                rate -=a
                wait = 1./rate
```

```
                t+=wait

            conf=np.append(conf,[eta],axis=0)
            nextout+=deltat
            bulk=np.append(bulk,N-eta[0])
            cond=np.append(cond,eta[0])
            times=np.append(times,t)


        tau.append(times/L)
        slow.append(cond/L)
        non_slow.append(bulk/L)


#slove numerically pdv
def firstorder(g,t):
    dgdt = c/L - (g/(g+1))/L - a*g
    return dgdt

markf = int(len(slow[len(Li)-1]))
t = np.linspace(0, 10*L, 10001)
g = odeint(firstorder,1,t)
f = np.zeros(len(t))
for i in range(len(t)):
    f[i] = rho*np.exp(-a*t[i]) -g[i]
    if f[i] < 0:
        f[i] = 0
        flipvalue = g[i]
        flipnumber = i
        break

for i in range(flipnumber, len(t)):
    g[i] = flipvalue * np.exp(-a*t[(i-flipnumber)])

for x in range(len(Li)):
    Lt = Li[x]
    plt.plot(tau[x], slow[x], markevery=markf, label = 's ' + str(Lt))
plt.plot(t/L, f, markevery=markf, label=('h(t)'))


for x in range(len(Li)):
    Lt = Li[x]
    plt.plot(tau[x], non_slow[x], markevery=markf, label = 'b ' + str(Lt))
plt.plot(t/L, g, markevery=markf, label=('g(t)'))

plt.legend()

plt.show()
```

and with another plot to make the second graph

```
    for x in range(len(Li)):
    Lt = Li[x]
   plt.plot(tau[x], np.log(slow[x] + non_slow[x]) , markevery=markf, label = 'G+H' + str(Lt))
```

```
plt.legend()
plt.show()
```

B

Python code to simulate annihilating bosons in a 3D harmonic potential

These approximations are done using several sections of code for graph **??**:

```
    import numpy as npy
import math as m
import matplotlib.pyplot as mpl
import pip


def redis(rates, energies, n):
    dis = npy.zeros(len(energies))
    for s in range(len(energies)):
        if n != s:
            dis[s] = rates[n][s]*npy.exp((energies[n]-energies[s])/2)
    return(dis)


presO = 100 # order of magnetude to witch the higest energy state has to be non-
occupied
dtnorm = 0.004 #timestep relative to temperature = timestep at T=Tc0
Nps = [100]  # number of particles
Tre = npy.arange(0.1, 1.4 ,0.05)
gamma = 0.9404989725 #=g3(1)^-(1/3)
parts = npy.zeros(len(Tre))


#first determine some parameters
for alpha in range(len(Tre)):
    dt = dtnorm #* 1/npy.exp((1/Tre[alpha]))
    Np = 100 #Nps[alpha]
    bhw = 1/(Tre[alpha]*(Np**(1/3))*gamma) #=beta h_ omega
   Nsmac = int(npy.log(presO)/bhw)+1 # highest energy step taken into account
    Ns = Nsmac
    El = npy.zeros(Ns)
    Mult = npy.zeros(Ns)
    for x in range(Ns):
        Mult[x] = (x+1)*(x+2)/2
      El[x] = 2.404*x*bhw  # Define energy levenls of the states with respect to temperature. W
```

```
    # Define the transfer rates between different states (symetrisch)
    transR = npy.zeros([Ns, Ns])
    for i in range(Ns):
        for j in range(Ns):
            if i == j:
                transR[i][i] = 0
            else:
                transR[i][j] = dt/abs(i-j)**3


    # Transisions if state occupied
    transstep = npy.zeros([Ns, Ns])
    for i in range(Ns):
        transstep[i] = redis(transR,El,i)

    #we build an initial occupation of the system as a matrix
   #the likelyhood of a certain amount f particles to be in a state is represented using a
    ppins = npy.zeros([Ns, max([20, 2*Np])])
    ppins [0][Np] = 1
    for i in range(1,Ns):
        ppins[i][0] = 1

    equi = True
    loop = 0
    while equi:
        for k in range(25000):
            pold = ppins
            pnew = ppins
            for i in range(Ns):
                Pless = 0
                Pmore = 0
                for j in range(Ns):
                                Pmore = Pmore + (transstep[j][i] * (1 -
ppins[j][0]))*(Mult[j]/Mult[i])
                    Pless = Pless + transstep[i][j]*(Mult[j]/Mult[i])
                x = npy.append(ppins[i][1:], 0)
                y = npy.insert(ppins[i][:-1],0,0)

                if True: #else:
                pnew[i][1:-1] = (1-Pless-Pmore)*ppins[i][1:-1] + Pless*x[1:-
1] + Pmore*y[1:-1]
                pnew[i][0] = (1-Pmore)*ppins[i][0] + Pless*x[0] + Pmore*y[0]
                          pnew[i][-1] = (1-Pless)*ppins[i][-1] + Pless*x[-
1] + Pmore*y[-1]
            ppins = pnew

        equi = False
        loop = loop +1
    print(loop)

    end = npy.zeros(Ns)
    for i in range(Ns):
        end[i] = sum(ppins[i])
```

```
    mean = npy.zeros(Ns)
    for i in range(Ns):
        ave = 0
        for j in range(2*Np):
            ave = ave + j * ppins[i][j]
        mean[i]= ave

    parts[alpha] = mean[0]/Np
    print(alpha)


mpl.plot(Tre, parts)

Tres = npy.arange(0, 1.5, 0.01)
Nres = npy.zeros(len(Tres))
for i in range(len(Tres)):
    Nres[i] = max(0, 1 - Tres[i]**3)

mpl.plot(Tres, Nres)

mpl.show()
```

Next the annihilation plot 3 sections of code are used so one step can be performed and checked at a time.

```
    import numpy as npy
import math as m
import matplotlib.pyplot as mpl
import pip
#import concurrent.futures as cf
#from numba import cuda, jit, njit, vectorize

#@cuda.jit(target = 'gpu')
def redis(rates, energies, n):
    dis = npy.zeros(len(energies))
    for s in range(len(energies)):
        if n != s:
            dis[s] = rates[n][s]*npy.exp((energies[n]-energies[s])/2)
    return(dis)


presO = 100 # order of magnetude to witch the higest energy state has to be non-
occupied
dtnorm = 0.004 #timestep relative to temperature = timestep at T=Tc0
Nps = [100] #[1, 3, 5, 10, 20, 40, 60, 100, 200, 300] # number of particles
Tre = [0.5]
DeltaE = 1/3 #difference between energy levels equivalent to particle density
gamma = 0.9404989725 #=g3(1)^-(1/3)
parts = npy.zeros(len(Tre))
acu = 100 #controls how many times the loop is run

#first determine some parameters
for alpha in range(len(Tre)):
    dt = dtnorm #* 1/npy.exp((1/Tre[alpha]))
    Np = 100 #Nps[alpha]
    bhw = 1/(Tre[alpha]*(Np**(1/3))*gamma) #=beta h_ omega
    Nsmac = int(npy.log(presO)/bhw) # highest energy step taken into account
```

```
    Ns = Nsmac


    # Define the transfer rates between different states (symetrisch)
    transR = npy.zeros([Ns, Ns])
    for i in range(Ns):
        for j in range(Ns):
            if i == j:
                transR[i][i] = 0
            else:
                transR[i][j] = dt/abs(i-j)**1

    El = npy.zeros(Ns)
    Mult = npy.zeros(Ns)
    for x in range(Ns):
        Mult[x] = (x+1)*(x+2)/2
     El[x] = 2.404*x*bhw  # Define energy levenls of the states with respect to temperatu

    # Transisions if state occupied
    transstep = npy.zeros([Ns, Ns])
    for i in range(Ns):
        transstep[i] = redis(transR,El,i)

    #we build an initial occupation of the system as a matrix
   #the likelyhood of a certain amount f particles to be in a state is represented using a
    ppins = npy.zeros([Ns, max([20, 2*Np])])
    ppins [0][Np] = 1
    for i in range(1,Ns):
        ppins[i][0] = 1

    equi = True
    loop = 0
    while equi:
        for k in range(30000):
            pold = ppins
            pnew = ppins
            for i in range(Ns):
                Pless = 0
                Pmore = 0
                for j in range(Ns):
                                Pmore = Pmore + (transstep[j][i] * (1 -
ppins[j][0]))*(Mult[j]/Mult[i])
                    Pless = Pless + transstep[i][j]*(Mult[j]/Mult[i])
                x = npy.append(ppins[i][1:], 0)
                y = npy.insert(ppins[i][:-1],0,0)

                if True: #else:
               pnew[i][1:-1] = (1-Pless-Pmore)*ppins[i][1:-1] + Pless*x[1:-
1] + Pmore*y[1:-1]
                pnew[i][0] = (1-Pmore)*ppins[i][0] + Pless*x[0] + Pmore*y[0]
                          pnew[i][-1] = (1-Pless)*ppins[i][-1] + Pless*x[-
1] + Pmore*y[-1]
            ppins = pnew
        equi = False

npy.save('quiTdTc0,5.npy', ppins)
```

```
import numpy as npy
import math as m
import matplotlib.pyplot as mpl
import pip

#import concurrent.futures as cf
#from numba import cuda, jit, njit, vectorize

#@cuda.jit(target = 'gpu')
def redis(rates, energies, n):
    dis = npy.zeros(len(energies))
    for s in range(len(energies)):
        if n != s:
            dis[s] = rates[n][s]*npy.exp((energies[n]-energies[s])/2)
    return(dis)


presO = 100 # order of magnetude to witch the higest energy state has to be non-
occupied
dtnorm = 0.004 #timestep relative to temperature = timestep at T=Tc0
Nps = [100] #[1, 3, 5, 10, 20, 40, 60, 100, 200, 300] # number of particles
Tre = [0.5]  #npy.arange(0.1, 1.2 ,0.1)
DeltaE = 1/3 #difference between energy levels equivalent to particle density
gamma = 0.9404989725 #=g3(1)^-(1/3)
parts = npy.zeros(len(Tre))
acu = 100 #controls how many times the loop is run

# add an anhillation therm with speed over exponential range compared to the speed at witch par
anhir = [0.001, 0.01/3, 0.01, 0.1/3, 0.1, 1/3, 1]
internloops = [30, 10, 3, 1, 1, 1, 1] #anhilation is only used every so many loops to reduce com
anhi = npy.zeros(len(anhir))
for i in range(len(anhir)):
    anhi[i] = anhir[i] * internloops[i]

Np = 100
bhw = 1/(Tre[0]*(Np**(1/3))*gamma) #=beta h_ omega
Nsmac = int(npy.log(presO)/bhw) # highest energy step taken into account
Ns = Nsmac
means = npy.zeros([len(anhi), Ns])


#first determine some parameters
for alpha in range(len(anhi)):
    dt = dtnorm #* 1/npy.exp((1/Tre[alpha]))
    Np = 100 #Nps[alpha]


   # Define energy levenls of the states with respect to temperature, El = E/2KbT

    # Define the transfer rates between different states (symetrisch)
    transR = npy.zeros([Ns, Ns])
    for i in range(Ns):
        for j in range(Ns):
```

```
            if i == j:
                transR[i][i] = 0
            else:
                transR[i][j] = dt/abs(i-j)**1

    El = npy.zeros(Ns)
    Mult = npy.zeros(Ns)
    for x in range(Ns):
        Mult[x] = (x+1)*(x+2)/2
     El[x] = 2.404*x*bhw  # Define energy levenls of the states with respect to temperatu

    # Transisions if state occupied
    transstep = npy.zeros([Ns, Ns])
    for i in range(Ns):
        transstep[i] = redis(transR,El,i)

    #we build an initial occupation of the system as a matrix
   #the likelyhood of a certain amount f particles to be in a state is represented using a
    maxp = max([20, 2*Np])
    ppins = npy.load('quiTdTc0,5.npy')

   anhil = anhi[alpha]*sum(transstep[0]) #calculating actual anhilation rates
   # anhilation first build a matrix 2Np such that for a number of particles in an orbit wi
    anhredis = npy.zeros([maxp, maxp])
    for i in range(maxp):
        for j in range (i+1):
            anhredis[i][j] = (m.comb(i,j))*((1-anhil)**j) * (anhil**(i-j))



    loop = 0
    means = npy.zeros([350, Ns])
    for time in range(350):
        loop = loop +1
        for k in range(int(1/anhi[alpha])):
            for sub in range(internloops[alpha]):
                pnew = ppins +0
                for i in range(Ns):
                    Pless = 0
                    Pmore = 0
                    for j in range(Ns):
                                Pmore = Pmore + (transstep[j][i] * (1 -
ppins[j][0]))*(Mult[j]/Mult[i])
                        Pless = Pless + transstep[i][j]*(Mult[j]/Mult[i])
                    x = npy.append(ppins[i][1:], 0)
                    y = npy.insert(ppins[i][:-1],0,0)


                    if True: #else:
                              pnew[i][1:-1] = (1-Pless-Pmore)*ppins[i][1:-
1] + Pless*x[1:-1] + Pmore*y[1:-1]
                 pnew[i][0] = (1-Pmore)*ppins[i][0] + Pless*x[0] + Pmore*y[0]
                           pnew[i][-1] = (1-Pless)*ppins[i][-1] + Pless*x[-
1] + Pmore*y[-1]

                pold = ppins +0
```

```
                ppins = pnew+0

            #anhilation
            for n in range(Ns):
                if ppins[n][0]> 0.9:
                    for j in range (maxp-1):
                pnew[n][j] = ppins[n][j]*(1- min(1, anhil*j) ) + ppins[n][j+1] * min(1, anhil
                else:
                    for j in range (maxp):
                        newlist = 0
                        for k in range (maxp):
                            newlist = newlist + ppins[n][k]*anhredis[k][j]
                        pnew[n][j] = newlist
            ppins = pnew+0
        print(loop)

        for i in range(Ns):
            ave = 0
            for j in range(2*Np):
                ave = ave + (j * pold[i][j])*Mult[i]
            means[time][i]= ave

    #save means for this anhilation rate
    data = npy.asarray(means)
   npy.save('anhilationrange_from_equi0.5' + str(int(1/anhir[alpha])) + '.npy', data)
```

```
import numpy as npy
import matplotlib as mpl
import matplotlib.pyplot as plt

#list all the files we want to plot

rates = [0.001, 0.01/3, 0.01, 0.1/3, 0.1, 1/3, 1]

for alpha in range(len(rates)):
    rates[alpha] = str(int(1/rates[alpha]))

fig, (ax1, ax2) = plt.subplots(1, 2)

for alpha in range(len(rates)):
    means = npy.load('anhilationrange_from_equi0.5' + rates[alpha] + '.npy')
    means2 = npy.zeros([350,10])
    for i in range(350):
        for j in range(10):
            means2[i][j] = means[i][j]* (j+1)*(j+2)/2
    N0 = npy.zeros(len(means2))
    N1 = npy.zeros(len(means2))
    Ntot = npy.zeros(len(means2))
    for t in range(len(means)):
        N0[t] = means2[t][0]
        N1[t] = sum(means2[t])-means2[t][0]
        Ntot[t] = sum(means2[t])
```

```
    ax1.plot(Ntot, N0)
    ax2.plot(Ntot, N1)

ax1.set_ylim(0,100)
ax1.set_xlim(100,0)
ax2.set_xlim(100,0)

plt.show()
```