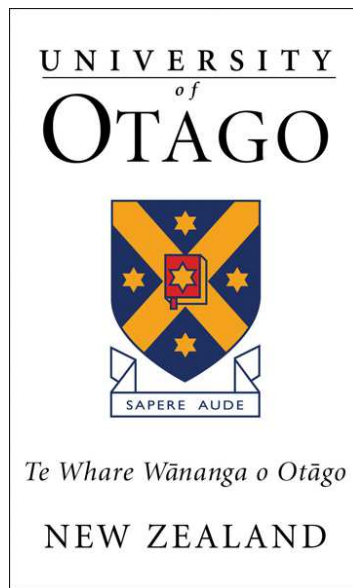


C-Field Theory of Dynamics in One Dimensional Bose Gases: The Kibble-Zurek Mechanism and Bright Soliton Arrest

Rob G. McDonald



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Abstract

A grand canonical $\mathbf{C}$ -field theory has been previously developed for modelling finite temperature Bose gases, the stochastic projected Gross-Pitaevskii equation (SPGPE) [1]. Previous investigations have shown quantitative agreement between experiments and the SPGPE, with a fitted growth rate [2, 3] or no fitted parameters at all [4]. These and other works [5, 6] have used the number-damping SPGPE, a sub-theory of the SPGPE neglecting a scattering process between the coherent and incoherent regions that conserves the particle number of each region, known as energy-damping. The systems in these works were in quasi-equilibrium and as such a growth process, also known as number-damping, is thought to be dominant. Evidence suggests that energy-damping is significant when the system is far from equilibrium [7]; we may also postulate systems where energy-damping is the only allowed process. In this thesis we use the full SPGPE including the energy-damping reservoir interaction in systems where this process plays an important role in the dissipative evolution.

We model quenches of chemical potential across the Bose-Einstein condensation transition in a one dimensional Bose gas confined to a toroid. We use two different models; the full SPGPE and the number-damping SPGPE. The purpose of this is to test the results of our simulations against the predictions of the Kibble-Zurek mechanism (KZM), a theory of defect formation in second order phase transitions. We find that both models give results consistent with KZM, in that various measurable quantities obey a power law with respect to the quench time. The power law exponents are determined by critical exponents, which depend on the universality class of the phase transition. We find the number-damping SPGPE results are consistent with the critical exponents predicted by mean field theory. We are unable to find a universality class with critical exponents consistent with the results of the full theory, and in particular the dynamical critical exponent differs from that predicted by mean field theory.

We also use the SPGPE to simulate the motion of a bright soliton in a one dimensional attractive Bose gas confined to a toroid and in contact with a thermal cloud of a second component. The bright soliton is an analytical solution of the one-dimensional Gross-Pitaevskii equation for an attractive Bose-Einstein condensate, which can propagate in space without changing its functional form. We derive a stochastic differential equation for the soliton velocity, finding that the energy-damping reservoir interaction manifests as an Ornstein-Uhlenbeck process for velocity decay, affording a complete analytic solution for the damping and diffusion rates of the bright soliton. The results of simulating the bright soliton using the SPGPE are compared against the analytic solutions of the velocity stochastic differential equation, including the mean, variance, two-time correlations, and power spectra of the velocity. We find that the numerical and analytical solutions show excellent agreement for all these quantities, validating our procedure for obtaining the velocity equation of motion.

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Chapter 1

Introduction

1.1 Overview

The successful creation of a Bose-Einstein condensate in a dilute alkali gas in 1995 [8] set off significant experimental and theoretical efforts in the field of ultra-cold gases. While this initial condensate was formed using repulsive bosons, a Bose-Einstein condensate of attractive bosons [9] was achieved later in the same year. The diluteness of the atoms in the gas mean that the required temperature to observe Bose-Einstein condensation is on the order of 10^{-5} K or less.

Dilute gas Bose-Einstein condensates provide an experimental platform where many of the system parameters can be controlled to a high degree of precision, giving excellent opportunities for theories to be compared directly to experiments. The Gross-Pitaevskii equation [10,11] is the most commonly used tool for the description of Bose-Einstein condensates, where the condensate itself is described by a single wave function. The Gross-Pitaevskii equation is a mean-field theory that describes coherent evolution of the condensate wave function while neglecting quantum fluctuations, and is a good approximation when all of the particles in the system are contained in the condensate. Thus the Gross-Pitaevskii equation may be used very successfully to give a quantitative description of condensates in the zero temperature regime. However experiments are commonly performed at finite temperature, where a significant thermal cloud gives rise to spontaneous and incoherent processes that cannot be described by the Gross-Pitaevskii equation.

In sufficiently high temperature Bose-Einstein condensates there exists coupling between the condensate mode and the thermal modes of the system that cannot be neglected. Including the various scattering processes that occur between the low-energy system modes, including the condensate mode, and high-energy modes leads to a stochastic theory known as the stochastic projected Gross-Pitaevskii equation (SPGPE), the basis of which lies in the $\mathbf{C}$ -field formalism [12]. The derivation and formalism of the SPGPE may be found in detail elsewhere [1,13]. The SPGPE provides a non-perturbative quantum description of all highly

occupied low energy modes of a Bose gas, as opposed to only the condensate itself. Other treatments either only consider the condensate mode in the quantum mechanical sense, or neglect the higher energy modes that form a thermal reservoir [14].

The SPGPE has been applied to spontaneous vortex formation during Bose-Einstein condensation [5] showing agreement with experiment, however the damping rate had to be determined by fitting to the experimental data for the condensate population. The theory has also been used to make quantitative predictions of single vortex decay [6] without any fitting parameters. For systems where a high energy fraction is approximately thermalised, the SPGPE is able to make quantitative predictions of the dynamics of finite temperature Bose gases without any fitting parameters for comparison to experiments. In an experiment on the formation of persistent currents in the high temperature regime [15], the damped Gross-Pitaevskii equation was used to model the experiment, with the model giving qualitative agreement. More recently, the same experiment was numerically reproduced using the SPGPE with no fitting parameters [4], with both short time dynamics and steady state values showing quantitative agreement.

The Kibble-Zurek mechanism [16] is a theory that describes the formation of topological defects in a system crossing a second order phase transition. There is a symmetry-breaking associated with crossing the transition point, where a specific phase must be ‘chosen’ in domains of finite size throughout the system. Thus domains of independently assigned phases form; to do otherwise would require communication of information across the entire system simultaneously, violating causality. The merging of domains with independent phases causes topological defects to form where there is a discrepancy in the phase. The Kibble-Zurek mechanism makes a prediction for the number of topological defects forming at a given finite quench rate, and in particular, the way the defect number scales with quench rate. This theory can be applied to the Bose-Einstein condensation transition, which takes place at a non-zero temperature and hence is poorly described using the Gross-Pitaevskii equation. Non-equilibrium dynamics are also inherently present during the transition due to critical slowing down; in the vicinity of the critical point, the system is unable to maintain equilibrium with the quenched thermal cloud. This mechanism is thus a good candidate for modelling using the SPGPE. In particular, it is an opportunity to probe the effect of including energy-damping on the system dynamics. Given that these processes should be significant for non-equilibrium systems, we can expect a significant correction to the number-damping sub-theory of the SPGPE.

Bright solitons were first observed in attractive Bose gases in 2002 [17], and their dynamics have been extensively studied in the ultra-cold regime where the thermal fraction is essentially negligible [18]. The system of a bright soliton embedded in a thermal cloud can be described using the SPGPE with appropriate approximations. If one neglects the number-damping process in the SPGPE, the energy-damping SPGPE is obtained; this sub-theory doesn’t

allow growth of the $\mathbf{C}$ -field particle number, and thus a bright soliton can exist as a stable quasi-particle without condensate collapse occurring. In this model, the bright soliton exists as the wave function one component, while a second component acts as a thermal bath. The dynamics of a bright soliton containing a constant number of particles can be entirely parametrised by its velocity. This system is thus a good candidate for testing a stochastic equation of motion for the soliton velocity.

1.2 Research Aims

The two main aims of this research are as follows:

1. To simulate quenches across the Bose-Einstein condensation transition in a repulsive Bose gas using both the full one-dimensional SPGPE and the one-dimensional number-damping SPGPE, and compare the results to the predictions of the Kibble-Zurek mechanism.
2. To obtain and test a stochastic differential equation for the velocity of a bright soliton in an attractive Bose gas immersed in a non-condensed thermal reservoir of a second component. The procedure involves using functional calculus to change variables from an equation of motion for the wave function (the SPGPE) to an equation of motion for a single parameter that defines the state of the system. The resulting equation is tested by comparing the analytic solutions to numerical solutions of the SPGPE.

1.3 Thesis Outline

We begin by giving some background on the fundamental properties of Bose-Einstein condensation, finite temperature theory, solitons and the Kibble-Zurek mechanism in chapter 2.

All of the work presented in this thesis is based on $\mathbf{C}$ -field treatments of the finite temperature Bose gas. In chapter 3 we give details of the formalism of $\mathbf{C}$ -field methods. The derivation of the SPGPE is outlined, and we present sub theories of the SPGPE including those neglecting certain scattering processes and systems with reduced dimensionality. In this thesis we consider systems where the $\mathbf{C}$ -field is one-dimensional in nature, while the thermal reservoir maintains three-dimensional characteristics. The systems also differ in the significance of the various scattering processes.

In chapter 4 we model quenches of chemical potential across the Bose-Einstein condensation transition for a one dimensional Bose gas confined to a toroidal geometry. We give details on the Kibble-Zurek mechanism, including derivations of the main predictions for our quench procedure. We model the quenches using both the full one dimensional SPGPE, and a sub-theory that neglects number-conserving scattering processes; the number-damping SPGPE.

The goal is to determine what effect, if any, the inclusion of these processes has on the way topological defect formation depends on the quench rate. We find that both theories give results that agree with the power law behaviour predicted by the Kibble-Zurek mechanism. However the two theories give differing power laws, with the number-damping SPGPE giving results that are in agreement with mean field theory. A universality class giving agreement with the full theory results could not be found, however the results indicate that the number-conserving scattering process may yet be important for determining the dynamical critical exponent.

In chapter 5 we present our derivation of a stochastic differential equation for the velocity of a bright soliton in a one dimensional attractive Bose gas confined to a toroidal geometry, and immersed in a non-condensed thermal reservoir of a second component. In this system energy-damping is the only allowed process, and as such we use the one-dimensional energy-damping SPGPE. Ito calculus is used to obtain a change of variables rule from the equation for the wave function to an equation for the velocity. The resulting equation describes an Ornstein-Uhlenbeck process, and the analytic solutions for the velocity are then presented. Simulations of a bright soliton in a finite temperature system are performed using the energy-damping SPGPE, and the results compared to the analytic solutions of the Ornstein-Uhlenbeck process. These show excellent agreement, validating our procedure for obtaining the stochastic differential equation for the velocity.

In chapter 6 we summarise the thesis and present the final conclusions. We also consider some possibilities for future research stemming from this investigation.

Chapter 2

Background

2.1 Bose-Einstein Condensation

The existence of Bose-Einstein condensates was first predicted by Einstein in 1924-25 [19, 20] based on work done by Bose in 1924 [21]. The statistics of an ideal (non-interacting) Bose gas at temperature T are described by the Bose-Einstein distribution

$$n_{BE}(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/k_B T} - 1} \quad (2.1)$$

where $n_{BE}(\epsilon)$ is the number of bosons occupying the state with energy ϵ , and the chemical potential μ constrains the total number of bosons in the gas. When a Bose gas is cooled to below a critical temperature T_c , a second-order phase transition occurs wherein the ground state of the gas becomes macroscopically occupied. The Bose-Einstein condensate is the portion of the gas occupying the ground state, and may be described as a coherent matter wave. For an infinite three dimensional ideal Bose gas, the critical temperature for condensation can be shown to be

$$T_c = \frac{2\pi\hbar^2}{mk_B} \left(\frac{n}{\zeta(3/2)} \right)^{2/3} \quad (2.2)$$

where $\zeta(x)$ is the Riemann zeta function and n is the particle density. External trapping and dimensional reduction lead to modifications of the critical temperature, as do interactions. In particular, the critical temperature for condensation in a harmonically trapped three dimensional ideal Bose gas is [10]

$$T_c = \frac{\hbar\bar{\omega}}{k_B} \left(\frac{N}{\zeta(3)} \right)^{1/3} \quad (2.3)$$

where $\bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$ is the geometric mean of the trapping frequencies and N is the number of particles. At zero temperature, an ideal Bose gas will have every particle occupying the

ground state, and the gas is said to be fully condensed.

The earliest evidence of Bose-Einstein condensation was the superfluidity of liquid helium; while superfluids and Bose-Einstein condensates are not identical, the two phenomena are related. When ^4He is cooled to below the lambda point ($T_\lambda = 2.17\text{K}$) a transition occurs where the liquid has many startling properties unlike those seen in a regular fluid [22, 23], such as non-dissipative flow. These can lead to such phenomena as persistent currents and quantised vortices, which have been well-studied. The strong interactions present in ^4He prevent an appreciably large condensate fraction from forming. This in turn makes study of the superfluid component properties difficult as the normal fluid component dominates.

The alkali gases have much weaker interactions than in ^4He , and thus much higher condensate fractions may be achieved. The low atomic densities of these gases result in the critical temperature also being very low, on the order of millionths of a Kelvin, a requirement that prevented the realisation of condensates until new cooling methods were developed. A gaseous Bose-Einstein condensate of rubidium-87 atoms was first created in 1995 [8] using a combination of laser cooling and evaporative cooling techniques to reach the extremely low temperature required, below 170 nK. This was quickly followed by the condensation of lithium-7 [9] and sodium-23 [24]. This development lead to much experimental and theoretical work in the field of ultra-cold atoms. Condensates in gases of molecules [25], photons [26], phonons [27] and other quasi-particles [28–30] have also been achieved.

2.1.1 Gross-Pitaevskii Equation

An appealing aspect of Bose-Einstein condensates is that there are valid approximations that may be made to the full many body quantum field theory to obtain more tractable theories. A commonly used theory describing a Bose-Einstein condensate is given by the Gross-Pitaevskii equation [10, 11]

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) + V(\mathbf{x}, t) \psi(\mathbf{x}, t) + g |\psi(\mathbf{x}, t)|^2 \psi(\mathbf{x}, t) \quad (2.4)$$

where $V(\mathbf{x}, t)$ is any external potential. This non-linear Schrodinger equation gives a mean-field description of a low temperature Bose-Einstein condensate, where the interactions between particles are well approximated as being contact interactions of the form

$$U(\mathbf{x} - \mathbf{x}') = g \delta(\mathbf{x} - \mathbf{x}'). \quad (2.5)$$

The parameter g determines the strength of the interactions and is related to the s-wave scattering length a_s by

$$g = \frac{4\pi a_s \hbar^2}{m}. \quad (2.6)$$

This may be positive or negative, resulting in a repulsive or attractive condensate respectively.

This theory gives an excellent description of condensate dynamics at zero-temperature [10], where every particle is condensed and can thus be represented by a single wave function, provided the gas is sufficiently dilute. The diluteness criteria is often stated as

$$n^{\frac{1}{3}}|a_s| \ll 1 \quad (2.7)$$

where n is the particle density. If this is not satisfied then quantum depletion of the condensate, a process not accounted for in the Gross-Pitaevskii equation [31], can be significant, even at zero temperature.

The Gross-Pitaevskii equation can also adequately describe condensates where the temperature is greater than zero but much less than the critical temperature, however in general the modelling of these finite temperature systems requires theories that include condensate and non-condensate dynamics, and their interactions.

2.1.2 Quantum Vortices

A prominent feature of Bose-Einstein condensates is the existence of the topological defects known as quantum or superfluid vortices. One may express the condensate wave function in terms of its density and phase

$$\psi(\mathbf{x}, t) = \sqrt{n(\mathbf{x}, t)} e^{i\theta(\mathbf{x}, t)} \quad (2.8)$$

and define the superfluid velocity as

$$\mathbf{v}(\mathbf{x}, t) = \frac{\hbar}{m} \nabla \theta(\mathbf{x}, t). \quad (2.9)$$

It is a well known identity in vector calculus that the curl of a gradient is zero, and thus the velocity field is rotationless everywhere in the condensate that the phase is defined. Furthermore, since the wave function is single-valued, the change in phase around any point in the condensate must be an integer multiple of 2π . If this phase change is non-zero, then the point in question has an undefined phase and thus the density must go to zero. These points represent quantum vortices, which act as carriers of quantised angular momentum in the condensate. Quantum vortices were first experimentally realised in Bose-Einstein condensates in 1999 [32].

In three dimensions, quantum vortices appear as lines of zero density within the fluid. These are hence often referred to as vortex lines, and can support wave-like excitations along their length. These excitations are known as Kelvin waves, and can lead to the decay of vortex lines into vortex rings. In two dimensions, quantum vortices manifest as points of zero density. In both three and two dimensions the role of quantum vortices in superfluid

turbulence is an active area of research [33–36]. Clearly superfluid vortices cannot exist in one dimension; the closest analogy is the black soliton, where there is a discontinuity in the condensate phase [37].

2.2 Finite Temperature Theory

While at very low temperatures the Gross-Pitaevskii equation is a sufficient theory, it neglects incoherent and thermal processes associated with interaction between the condensate mode and other modes. These processes become important when there is an appreciable thermal cloud. Zero temperature is unable to be reached experimentally, and temperatures far below the critical temperature are very difficult to access. Thus a theory is required that can describe the dynamics of a condensate in the higher temperature regime, where the interactions between the condensate mode and thermal modes are significant. This regime occurs when the thermal energy is significant compared to the energy of single particle modes in the external trapping potential. For a harmonic trap with frequency ω , this is equivalent to

$$\hbar\omega \ll k_B T, \quad (2.10)$$

which in three dimensions generally gives temperatures above $0.6T_c$. In this work we operate in or very close to this high temperature regime. To this end we use a stochastic projected Gross-Pitaevskii equation which is based on **C**-field techniques [12].

2.2.1 C-field Theory

The theory we choose to utilise is one of several that are generically referred to as **C**-field theories [12]. Within the high-temperature regime the lowest energy modes are still significantly occupied. When this occupation is greater than a single quantum the system is highly Bose degenerate, and hence the quantum field can be treated using a classical field. Quantum features are still contained in this description, thus the name **C**-field is used to avoid the perception that it is a purely classical treatment.

The **C**-field techniques involve the use of a projection operator, which divides the system into two subspaces defined by a high-energy cutoff where the occupation drops to less than a single quantum. The subspace below the cutoff consisting of the low energy modes with significant occupation is treated fully quantum mechanically using a classical field representation, while the subspace above the cutoff consisting of the higher energy modes is treated semi-classically as a thermal cloud.

The thermal cloud is treated as a thermal reservoir which couples to the atoms in the **C**-field [1, 12, 13]. A stochastic projected Gross-Pitaevskii equation may then be derived where the wave function represents all modes in the **C**-field rather than just the condensate. The effect of incorporating the thermal cloud is to introduce new terms into the Gross-Pitaevskii

equation, representing additional damping and noise. An overview of $\mathbf{C}$ -field theory and the stochastic projected Gross-Pitaevskii equation is given in the next chapter.

2.3 Solitons

Although superfluid vortices are not present in one dimensional systems, they can support other topological features known as solitons. Solitons are solitary waves that appear in systems where the medium supporting the waves includes a non-linearity, such as that in the Gross-Pitaevskii equation. The defining feature of a soliton is that it can propagate at constant velocity without changing its shape. This is due to a balance between the non-linearity and dispersive effects in the medium. Another curious property of solitons is that their size and shape is maintained even after interacting with another soliton, although there is a phase shift associated with this process [38].

A one dimensional Bose-Einstein condensate can support one of two types of soliton, depending on the sign of the s-wave scattering length a_s of the gas particles.

2.3.1 Bright Solitons

If the scattering length is negative then we say the Bose gas is attractive. While Bose-Einstein condensates can be made in attractive Bose gases, they are generally unstable and collapse if the number of particles in the condensate exceeds some critical value [10]. This is true in both three and two dimensions, however in one dimension a condensate may be maintained in a stable state with no theoretical upper bound on the number of particles [39,40]. However in practice there are no true one dimensional systems, and the approximation of a system as one dimensional will become less valid as the number of particles is increased, thus in experiments an effective upper bound to the particle number will exist.

In one dimension, an attractive Bose-Einstein condensate can support bright solitons [17]. These manifest as localised regions of high particle density. Due to the negative scattering length, it is energetically favourable for particles to ‘clump’ together. Thus having all of the particles contained within a bright soliton is a lower energy state than having uniform density in the condensate, and so the bright soliton is stable for constant particle number, provided it is less than the aforementioned upper bound. If this upper bound is exceeded the matter wave system becomes unstable against collapse.

2.3.2 Dark Solitons

If the scattering length is positive then we say the Bose gas is repulsive. Bose-Einstein condensates in repulsive gases exhibit far greater stability than their attractive counterparts. Unlike in attractive condensates there is no theoretical limit to the number of particles that can

be stably contained within a repulsive condensate without a collapse occurring [10]. However 2-body and 3-body losses will limit the possible number of particles in the condensate.

In one dimension, a repulsive Bose-Einstein condensate can support dark solitons [41]. These manifest as localised regions of low particle density relative to some background density, along with a spike in the gradient of the condensate phase. The terminology for dark solitons is slightly more varied than for bright solitons, with there being a distinction between moving and stationary solitons. Stationary dark solitons have a density minimum that reaches zero and are hence referred to as *black* solitons. Moving dark solitons have a non-zero minimum and are hence referred to as *grey* solitons. Unlike the bright solitons, dark solitons are unstable and in the presence of dissipation undergo decay via self-acceleration taking the system to the uniform density state.

The one dimensional Gross-Pitaevskii equation admits analytical solutions for both bright and dark solitons [42,43]. This can allow analytic progress to be made when considering Bose-Einstein condensates containing one of these two quasi-particles.

2.4 The Kibble-Zurek Mechanism

The Kibble-Zurek mechanism is a theory originally proposed to describe the emergence of topological defects during the formation of the early universe [44,45]. The theory by Kibble suggests that at some stage early in its evolution, the universe underwent a second order phase transition from a symmetric state to an asymmetric state, the asymmetry being characterised by the choice of a phase of the order parameter describing the universe. During the transition, all points in space must choose a phase independently; for all points to choose the same phase would imply transfer of information throughout the system instantaneously, thus violating causality. Domains of independent phase then form and grow throughout the system, and where these domains meet the discrepancy in phase results in topological defects such as domain walls and cosmic strings.

2.4.1 Condensed Matter Systems

The relevance of this process to condensed matter systems was realised by Zurek, in the context of liquid helium transitioning to a superfluid [46] as well as in superconductors [47,48]. The same reasoning leads to the prediction of vortex lines appearing during the transition. In particular, the importance of the rate at which the transition is crossed was discussed. It can be shown that the relationship between this quench rate τ_Q and the number of topological defects appearing in the system is given by a power law

$$n_D(\tau_Q) \propto \tau_Q^{\frac{\nu}{1+z\nu}} \quad (2.11)$$

where ν and z are the correlation length and dynamic critical exponents respectively. These critical exponents describe how various properties of the system behave as the transition point is approached. Suppose the phase of a system is characterised by the parameter λ , and a second order phase transition may be induced by driving λ across its critical value λ_c . Then the correlation length critical exponent ν describes the divergence of the correlation length

$$\xi \propto (\lambda - \lambda_c)^{-\nu} \quad (2.12)$$

while the product of the correlation length and dynamical critical exponents $z\nu$ describes the divergence of the relaxation time

$$\tau \propto (\lambda - \lambda_c)^{-z\nu} \quad (2.13)$$

in the vicinity of the transition.

The concept of universality is important in this theory, as many systems with second order phase transitions share the same critical exponents, despite differing in their microscopic details. Experimentally quenches can thus be used to find the values of these critical exponents and hence the universality class of the transition.

This theory can of course be applied to the Bose-Einstein condensation transition in gases [49], a second order phase transition. The types of defects that appear depends on the dimensionality of the system under consideration. In three dimensions the defects that appear are vortex lines, as in superfluid helium. In two dimensions vortices appear, while in one dimension dark solitons form [50].

Chapter 3

C-field Theory

3.1 Introduction

In a highly degenerate Bose system, the highly occupied modes of the system may be described by a classical field rather than using the full many body quantum field theory. Various methods used to describe these systems exploit this fact, and are thus known generally as **C**-field methods. In this chapter we give a general outline of the derivation of the **C**-field theory known as the stochastic projected Gross-Pitaevskii equation. The original formulation using this method can be found in [1]. The general procedure can also be found in the review [12], along with further details for all **C**-field techniques. A further generalisation to spinor and multicomponent systems can be found in [51].

3.2 Effective Field Theory

To model the dynamics or find the ground state of a Bose gas, we must in general start with the second-quantised Hamiltonian

$$\begin{aligned}\hat{H} = & \int d^3\mathbf{x} \hat{\Psi}^\dagger(\mathbf{x}, t) H_{sp} \hat{\Psi}(\mathbf{x}, t) \\ & + \frac{1}{2} \int d^3\mathbf{x} \int d^3\mathbf{x}' \hat{\Psi}^\dagger(\mathbf{x}, t) \hat{\Psi}^\dagger(\mathbf{x}', t) U(\mathbf{x} - \mathbf{x}') \hat{\Psi}(\mathbf{x}', t) \hat{\Psi}(\mathbf{x}, t)\end{aligned}\quad (3.1)$$

where the single particle Hamiltonian is of the form

$$H_{sp} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}, t) \quad (3.2)$$

with $V(\mathbf{x}, t)$ the external potential. The Bose field operator $\hat{\Psi}(\mathbf{x}, t)$ annihilates a particle at position $\mathbf{x}$ and time t , while its conjugate $\hat{\Psi}^\dagger(\mathbf{x}, t)$ creates a particle at position $\mathbf{x}$ and time t .

These field operators obey the Bosonic field commutation relations

$$[\hat{\Psi}(\mathbf{x}, t), \hat{\Psi}^\dagger(\mathbf{x}', t)] = \delta(\mathbf{x} - \mathbf{x}') \quad (3.3)$$

and

$$[\hat{\Psi}^\dagger(\mathbf{x}, t), \hat{\Psi}^\dagger(\mathbf{x}', t)] = [\hat{\Psi}(\mathbf{x}, t), \hat{\Psi}(\mathbf{x}', t)] = 0 \quad (3.4)$$

The two body interaction $U(\mathbf{x} - \mathbf{x}')$ generally has a finite range that is determined by the effective size of the atoms. Typically, the temperatures involved in Bose-Einstein condensation are low enough that the thermal de Broglie wavelength of the atoms extends beyond this range. We impose a high-energy cutoff $E_{\max}$, where all modes with energy greater than this are totally neglected, to define a new subspace $\mathbf{L}$. The low temperatures involved ensure that the occupancy of these modes is very low, so the interaction between them and the lower modes is negligible. Then we may approximate the two body interaction potential for the remaining modes to be of the contact type as it is in the Gross-Pitaevskii theory. The particle interactions are now entirely characterised by the s-wave scattering length, and we have a new effective field theory given by the Hamiltonian

$$\hat{H}_{\text{eff}} = \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}, t) H_{\text{sp}} \hat{\psi}(\mathbf{x}, t) + \frac{g}{2} \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t) \hat{\psi}(\mathbf{x}, t) \quad (3.5)$$

where the parameter g is related to the s-wave scattering length a_s by

$$g = \frac{4\pi a_s \hbar^2}{m}. \quad (3.6)$$

This effective field theory describes the coarse-grained field operator $\hat{\psi}(\mathbf{x}, t)$ that consists of the lower energy modes making up $\mathbf{L}$. This field operator can be represented as a sum over the single particle modes contained in $\mathbf{L}$

$$\hat{\psi}(\mathbf{x}, t) = \sum_{n \in \mathbf{L}} \phi_n(\mathbf{x}, t) \hat{a}_n \quad (3.7)$$

where $\phi_n(\mathbf{x}, t)$ are the single-particle eigenstates of H_{sp} with energy ϵ_n

$$H_{\text{sp}} \phi_n(\mathbf{x}, t) = \epsilon_n \phi_n(\mathbf{x}, t) \quad (3.8)$$

and $n \in \mathbb{N}$ represents the n th mode of the system starting with the lowest energy mode $n = 0$. The coarse-grained field operator also obeys the Bosonic field commutation relations with the

true Dirac delta function replaced by a coarse-grained delta

$$[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] = \delta_{\mathbf{L}}(\mathbf{x}, \mathbf{x}') = \sum_{n \in \mathbf{L}} \phi_n(\mathbf{x}) \phi_n^*(\mathbf{x}'). \quad (3.9)$$

The operator $\hat{a}_n$ removes a particle from the n th mode, while its conjugate $\hat{a}_n^\dagger$ adds a particle to the n th mode. These operators obey the commutation relations

$$[\hat{a}_n, \hat{a}_m^\dagger] = \delta_{nm} \quad (3.10)$$

and

$$[\hat{a}_n^\dagger, \hat{a}_m^\dagger] = [\hat{a}_n, \hat{a}_m] = 0. \quad (3.11)$$

These commutation relations allow one to find the Heisenberg equation of motion for the field operator

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{x}, t)}{\partial t} = \int d^3\mathbf{x}' \delta_{\mathbf{L}}(\mathbf{x}, \mathbf{x}') \left\{ H_{\text{sp}} \hat{\psi}(\mathbf{x}', t) + g \hat{\psi}^\dagger(\mathbf{x}', t) \hat{\psi}(\mathbf{x}', t) \hat{\psi}(\mathbf{x}', t) \right\}. \quad (3.12)$$

Solving this equation of motion is required to understand the dynamics of any Bose condensed system, however this is a highly non-trivial task. Fortunately, **C**-field techniques allow progress to be made in suitable regimes.

3.3 Projected Field Theory

3.3.1 Projection Operators

The modes represented by the effective field theory are divided into two further subspaces, defined by an energy cutoff ϵ_{cut} at which the modes have an occupation on the order of unity. The lower energy subspace is referred to as the coherent region **C**, while the higher energy subspace is the incoherent region **I**; this is demonstrated in Figure 3.1. The **C**-field consists of all modes that satisfy $\epsilon_n \leq \epsilon_{\text{cut}}$, while the **I**-field consists of all modes that satisfy $\epsilon_{\text{cut}} < \epsilon_n < E_{\text{max}}$. The effective field operators are decomposed as

$$\hat{\psi}(\mathbf{x}, t) = \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) + \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t). \quad (3.13)$$

The coherent field $\hat{\psi}_{\mathbf{C}}(\mathbf{x}, t)$ will be treated fully quantum mechanically, while the incoherent field $\hat{\psi}_{\mathbf{I}}(\mathbf{x}, t)$ will be considered to be essentially fully thermalised. Two projectors $\mathcal{P}$ and $\mathcal{Q}$ are defined with the former projecting into the coherent region **C** and the latter projecting into the incoherent region **I**. These projectors may be represented in the single particle mode

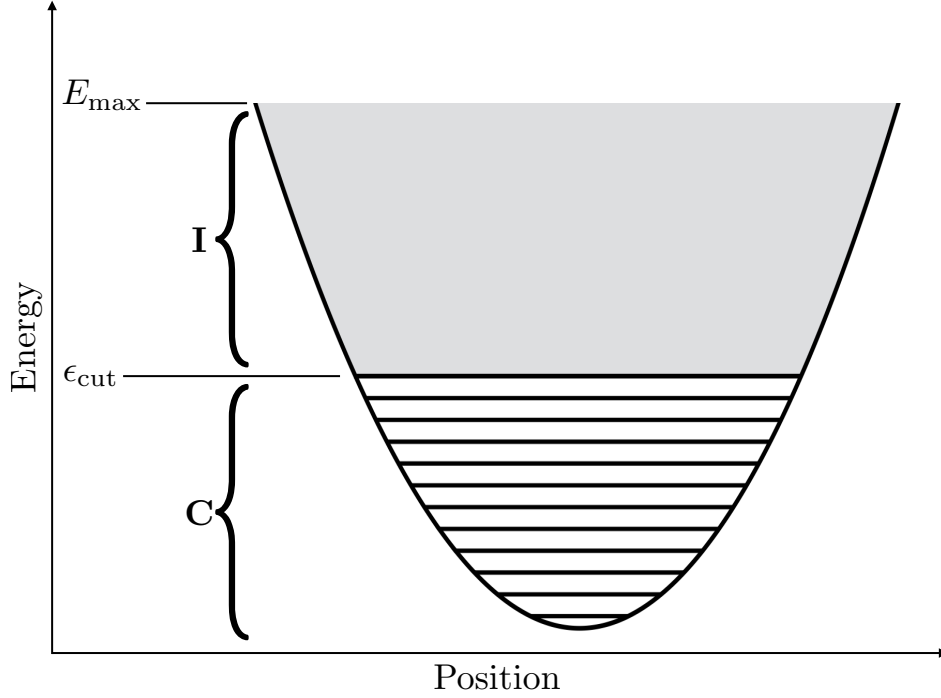


Figure 3.1: A schematic showing the coherent region **C**, incoherent region **I**, and states eliminated to give the effective field theory. In the stochastic Gross-Pitaevskii equation, the coherent region is treated quantum mechanically in a classical field approximation. The incoherent region is treated semi-classically, and is most simply described as a grand canonical reservoir.

basis as

$$\mathcal{P}\{F(\mathbf{x})\} = \sum_{n \in \mathbf{C}} \phi_n(\mathbf{x}) \int d^3\mathbf{x}' \phi_n^*(\mathbf{x}') F(\mathbf{x}') \quad (3.14)$$

and

$$\mathcal{Q}\{F(\mathbf{x})\} = \sum_{n \in \mathbf{I}} \phi_n(\mathbf{x}) \int d^3\mathbf{x}' \phi_n^*(\mathbf{x}') F(\mathbf{x}'). \quad (3.15)$$

In particular, applying the projectors to the effective field operator gives

$$\mathcal{P}\{\hat{\psi}(\mathbf{x}, t)\} = \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) \quad (3.16)$$

and

$$\mathcal{Q}\{\hat{\psi}(\mathbf{x}, t)\} = \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t). \quad (3.17)$$

Note that the composition of the projectors is zero

$$\mathcal{P} \{ \mathcal{Q} \{ F(\mathbf{x}) \} \} = \mathcal{Q} \{ \mathcal{P} \{ F(\mathbf{x}) \} \} = 0 \quad (3.18)$$

and their summation is equivalent to the identity operator

$$\mathcal{P} \{ F(\mathbf{x}) \} + \mathcal{Q} \{ F(\mathbf{x}) \} = F(\mathbf{x}) \quad (3.19)$$

After the projection, the commutator is no longer a pure Dirac delta, and is now given by

$$[\hat{\psi}_{\mathbf{C}}(\mathbf{x}, t), \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}', t)] = \delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x}') \quad (3.20)$$

where $\delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x}')$ is formally the kernel of the $\mathbf{C}$ region projector $\mathcal{P}$

$$\delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x}') = \sum_{n \in \mathbf{C}} \phi_n(\mathbf{x}) \phi_n^*(\mathbf{x}'). \quad (3.21)$$

Although not a true Dirac delta, this behaves identically to one within the $\mathbf{C}$ region, so for any function $F_{\mathbf{C}}(\mathbf{x})$ consisting only of modes in the $\mathbf{C}$ region

$$\int d^3 \mathbf{x}' \delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x}') F_{\mathbf{C}}(\mathbf{x}') = F_{\mathbf{C}}(\mathbf{x}). \quad (3.22)$$

3.3.2 Hamiltonian Decomposition

When we insert our effective field decomposition into the effective field Hamiltonian, we may write the result as

$$\hat{H}_{\text{eff}} = \hat{H}_{\mathbf{C}} + \hat{H}_{\mathbf{I}} + \hat{H}_{\mathbf{C}, \mathbf{I}} \quad (3.23)$$

where the $\hat{H}_{\mathbf{C}}$, $\hat{H}_{\mathbf{I}}$, and $\hat{H}_{\mathbf{C}, \mathbf{I}}$ refer to the terms in the Hamiltonian containing only the coherent field operator $\hat{\psi}_{\mathbf{C}}(\mathbf{x}, t)$, only the incoherent field operator $\hat{\psi}_{\mathbf{I}}(\mathbf{x}, t)$, and a mixture of both field operators respectively. The Hamiltonian for the $\mathbf{C}$ and $\mathbf{I}$ region interactions is further decomposed into

$$\hat{H}_{\mathbf{C}, \mathbf{I}} = \hat{H}_{\mathbf{C}, \mathbf{I}}^{(1)} + \hat{H}_{\mathbf{C}, \mathbf{I}}^{(2)} + \hat{H}_{\mathbf{C}, \mathbf{I}}^{(3)} \quad (3.24)$$

where the numbers in the superscripts refer to how many times the coherent region operator $\hat{\psi}_{\mathbf{C}}(\mathbf{x}, t)$ appears in each term. The individual terms of the effective field Hamiltonian are

$$\hat{H}_{\mathbf{C}} = \int d^3 \mathbf{x} \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}, t) H_{sp} \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) + \frac{g}{2} \int d^3 \mathbf{x} \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) \quad (3.25)$$

$$\hat{H}_{\mathbf{I}} = \int d^3 \mathbf{x} \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) H_{sp} \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t) + \frac{g}{2} \int d^3 \mathbf{x} \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t) \quad (3.26)$$

$$\hat{H}_{\mathbf{C},\mathbf{I}}^{(1)} = g \int d^3\mathbf{x} \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) + \text{h.c.} \quad (3.27)$$

$$\begin{aligned} \hat{H}_{\mathbf{C},\mathbf{I}}^{(2)} = & 2g \int d^3\mathbf{x} \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) \\ & + \frac{g}{2} \int d^3\mathbf{x} \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) + \text{h.c.} \end{aligned} \quad (3.28)$$

$$\hat{H}_{\mathbf{C},\mathbf{I}}^{(3)} = g \int d^3\mathbf{x} \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}, t) \hat{\psi}_{\mathbf{C}}(\mathbf{x}, t) \hat{\psi}_{\mathbf{I}}(\mathbf{x}, t) + \text{h.c.} \quad (3.29)$$

where h.c. denotes the Hermitian conjugate. The terms involving the single particle Hamiltonian and one each of $\hat{\psi}_{\mathbf{C}}(\mathbf{x}, t)$ and $\hat{\psi}_{\mathbf{I}}(\mathbf{x}, t)$ vanish due to the orthogonality of the single-particle modes in each region.

3.3.3 C-field Theories

At this point one may access several different **C**-field theories based on the treatment of the interaction Hamiltonian $\hat{H}_{\mathbf{C},\mathbf{I}}$, which contains field operators of both the **C**-field and **I**-field.

The projected Gross-Pitaevskii equation (PGPE) is simply the Gross-Pitaevskii equation applied to the **C**-field wave function, with the addition of the **C**-field projector. All terms in the interaction Hamiltonian are neglected, and hence no coupling between the **C**-field and **I**-field is accounted for. In this theory, the **C**-field is treated as a microcanonical system with fixed energy and particle number.

The stochastic projected Gross-Pitaevskii equation (SPGPE) retains all the interaction terms, and hence takes into account the scattering processes occurring between particles in the **C**-field and particles in the **I**-field. The scattering processes are implemented in theory by finding a stochastic differential equation with multiple dissipative and stochastic noise terms. This results in a more complex equation than the PGPE. Since the SPGPE includes interactions between the **C**-field and **I**-field, occupation of the **I**-field can be accounted for. Thus this theory is suitable for temperatures much higher than the single particle energy, where there is a significant thermal component.

The truncated Wigner projected Gross-Pitaevskii equation (TWGPE) is a useful theory for when there exists modes in the **C**-field with high occupation. This allows the use of approximations with respect to the interaction terms, giving a more tractable equation of motion. While the equation of motion for this model appears superficially similar to the PGPE, it differs by the inclusion of extra noise to account for quantum fluctuations. These quantum fluctuations can be approximated by sampling the initial Wigner distribution. This theory allows the description of non-equilibrium dynamics of Bose-Einstein condensates at very low temperatures $T \ll T_c$, at a level beyond mean-field.

In terms of describing high temperature Bose-Einstein condensates, the SPGPE gives the most complete description of the system due to its treatment of scattering processes with thermally occupied modes. The SPGPE is an extension of the PGPE, and also relies on the truncated Wigner approximation, thus it is necessary to consider these in the formulation of the SPGPE theory.

3.4 Wigner Formalism

The **C**-field methods involve choosing an energy cutoff ε_{cut} such that all modes in the coherent region are significantly occupied. Thus the system is highly quantum degenerate and may be treated using a classical field description. The quantum mechanical nature of the system is still expressed, however, through the interpretation of the classical variables. This is done by mapping the time evolution of the density operator to a classical quasi-probability function known as the Wigner function. The equation of motion for the quasi-probability distribution can then be further mapped to an equivalent stochastic differential equation. This is in general much easier to solve than the full quantum problem, which inevitably involves a large Hilbert space. A detailed background of phase space methods and the Wigner representation of quantum fields may be found in [52].

3.4.1 Coherent States

In some sense, the property $\hbar \neq 0$ is what defines a quantum description of a system. If one takes the limit $\hbar \rightarrow 0$ then a classical description of the system dynamics should be obtained. However, in some quantum systems this limit does not correspond to classical motion. Instead, one must find states of minimum uncertainty $|\alpha\rangle$, which then have properties that are the closest to classical of any quantum state. It can be shown that these minimum uncertainty states satisfy

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \quad (3.30)$$

where $\hat{a}$ is the annihilation operator, α is complex, and the states $|\alpha\rangle$ are known as coherent states. The coherent states form an overcomplete basis, and thus any general state can be written as a weighted sum over them. Coherent states appear frequently when using phase space methods, and are an important tool in the description of Bose gases.

3.4.2 Single Mode

If a quantum system is in a mixed state, a statistical ensemble of states $|\psi_i\rangle$, then the density operator of the system is defined as

$$\hat{\rho}(t) = \sum_i p_i |\psi_i, t\rangle \langle \psi_i, t| \quad (3.31)$$

where p_i is the probability that the system is found to be in the state $|\psi_i, t\rangle$.

Phase space methods rely on expressing the density operator in terms of a function of the coherent state eigenvalue α . The Wigner representation does this through the Wigner function [53], which expresses the density operator on the basis of coherent states. The Wigner function is defined as the Fourier transform of the symmetrically ordered quantum characteristic function

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2} \int d^2\lambda \exp[-\lambda\alpha^* + \lambda^*\alpha] \chi(\lambda, \lambda^*) \quad (3.32)$$

where the symmetrically ordered quantum characteristic function is given by

$$\chi(\lambda, \lambda^*) = \text{tr} \left\{ \hat{\rho} \exp \left[\lambda \hat{a}^\dagger - \lambda^* \hat{a} \right] \right\}. \quad (3.33)$$

The Wigner function exists for any given density operator, thus it is always possible to get a function of α if a density operator is defined. The key to phase space methods is the ability to map the action of a quantum operator on the density operator to the action of a differential operator on the Wigner function. The following operator correspondences exist for the actions of the creation and annihilation operators on the density operator [52]

$$\hat{a}\hat{\rho} \longleftrightarrow \left(\alpha + \frac{1}{2} \frac{\partial}{\partial \alpha^*} \right) W(\alpha, \alpha^*) \quad (3.34)$$

$$\hat{a}^\dagger \hat{\rho} \longleftrightarrow \left(\alpha^* - \frac{1}{2} \frac{\partial}{\partial \alpha} \right) W(\alpha, \alpha^*) \quad (3.35)$$

$$\hat{\rho}\hat{a} \longleftrightarrow \left(\alpha - \frac{1}{2} \frac{\partial}{\partial \alpha^*} \right) W(\alpha, \alpha^*) \quad (3.36)$$

$$\hat{\rho}\hat{a}^\dagger \longleftrightarrow \left(\alpha^* + \frac{1}{2} \frac{\partial}{\partial \alpha} \right) W(\alpha, \alpha^*) \quad (3.37)$$

These operator correspondences define the mapping from the evolution of the density operator to that of the Wigner function for the case of a single quantum mode. To describe our system

we need to extend the representation to multiple modes.

3.4.3 Quantum Field

For a system of M modes in the coherent region, the multimode Wigner function is given by [12]

$$W_{\mathbf{C}}(\boldsymbol{\alpha}, \boldsymbol{\alpha}^*) = \int \frac{d^2 \boldsymbol{\lambda}}{\pi^{2M}} \exp(\boldsymbol{\lambda}^* \boldsymbol{\alpha} - \boldsymbol{\alpha}^* \boldsymbol{\lambda}) \chi(\boldsymbol{\lambda}, \boldsymbol{\lambda}^*) \quad (3.38)$$

where $\boldsymbol{\alpha}$ is defined as the vector of mode amplitudes $\boldsymbol{\alpha} = [\alpha_0, \alpha_1, \dots, \alpha_{M-1}]$, $\chi(\boldsymbol{\lambda}, \boldsymbol{\lambda}^*)$ is the symmetric quantum characteristic function for the coherent region density operator $\hat{\rho}_{\mathbf{C}}$

$$\chi(\boldsymbol{\lambda}, \boldsymbol{\lambda}^*) = \text{tr} \left\{ \hat{\rho}_{\mathbf{C}} \exp \left[\sum_{n \in \mathbf{C}} (\lambda_n \hat{a}_n^\dagger - \lambda_n^* \hat{a}_n) \right] \right\}, \quad (3.39)$$

and where

$$\int d^2 \boldsymbol{\alpha} \equiv \prod_{n \in \mathbf{C}} \int d^2 \alpha_n. \quad (3.40)$$

One can then expand the classical field wave function over the single-particle states using the mode amplitudes

$$\psi_{\mathbf{C}}(\mathbf{x}) = \sum_{n \in \mathbf{C}} \alpha_n \phi_n(\mathbf{x}). \quad (3.41)$$

To look at the classical field average, one can use the fact that moments of the Wigner distribution give symmetrically ordered operator averages. The field density average is then

$$\begin{aligned} \int d^2 \boldsymbol{\alpha} |\psi_{\mathbf{C}}(\mathbf{x})|^2 W_{\mathbf{C}}(\boldsymbol{\alpha}, \boldsymbol{\alpha}^*) &= \left\langle \frac{\hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}) \hat{\psi}_{\mathbf{C}}(\mathbf{x}) + \hat{\psi}_{\mathbf{C}}(\mathbf{x}) \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x})}{2} \right\rangle \\ &= \langle \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}) \hat{\psi}_{\mathbf{C}}(\mathbf{x}) \rangle + \frac{\delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x})}{2}. \end{aligned} \quad (3.42)$$

The extra term containing $\delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x})$ arises from the commutator of the field operators, and refers to the presence of vacuum noise. This accounts for half a quantum per mode of noise, and shows that quantum effects are still present in the Wigner representation.

Once again, operator correspondences can be derived between the density operator and the Wigner function. The multimode calculations can be simplified by defining the projected functional derivative operators

$$\frac{\bar{\delta}}{\bar{\delta} \psi_{\mathbf{C}}(\mathbf{x})} \equiv \sum_{n \in \mathbf{C}} \phi_n^*(\mathbf{x}) \frac{\partial}{\partial \alpha_n}, \quad (3.43)$$

$$\frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} \equiv \sum_{n \in \mathbf{C}} \phi_n(\mathbf{x}) \frac{\partial}{\partial \alpha_n^*} \quad (3.44)$$

where the barred deltas indicate that the operation is projected. Using these projected functional derivatives, one may find the operator correspondences between $\hat{\rho}_{\mathbf{C}}$ and the Wigner function

$$\hat{\psi}_{\mathbf{C}}(\mathbf{x}) \hat{\rho}_{\mathbf{C}} \longleftrightarrow \left(\psi_{\mathbf{C}}(\mathbf{x}) + \frac{1}{2} \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} \right) W_{\mathbf{C}} \quad (3.45)$$

$$\hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}) \hat{\rho}_{\mathbf{C}} \longleftrightarrow \left(\psi_{\mathbf{C}}^*(\mathbf{x}) - \frac{1}{2} \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} \right) W_{\mathbf{C}} \quad (3.46)$$

$$\hat{\rho}_{\mathbf{C}} \hat{\psi}_{\mathbf{C}}(\mathbf{x}) \longleftrightarrow \left(\psi_{\mathbf{C}}(\mathbf{x}) - \frac{1}{2} \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} \right) W_{\mathbf{C}} \quad (3.47)$$

$$\hat{\rho}_{\mathbf{C}} \hat{\psi}_{\mathbf{C}}^\dagger(\mathbf{x}) \longleftrightarrow \left(\psi_{\mathbf{C}}^*(\mathbf{x}) + \frac{1}{2} \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} \right) W_{\mathbf{C}} \quad (3.48)$$

These operator correspondences are used to map the equation of motion for $\hat{\rho}_{\mathbf{C}}$ to an equivalent equation of motion for the $\mathbf{C}$ -field Wigner function $W_{\mathbf{C}}$.

3.4.4 Truncated Wigner Approximation

The Hamiltonian evolution of the $\mathbf{C}$ -field density operator is given by von Neumann's equation

$$i\hbar \partial_t \hat{\rho}_{\mathbf{C}}(t) = [\hat{H}_{\mathbf{C}}, \hat{\rho}_{\mathbf{C}}(t)] \quad (3.49)$$

where we have ignored the interactions between the coherent and incoherent regions. Due to the large Hilbert space involved, solving this equation is a difficult task, so the operator correspondences are used to map it to an equivalent evolution equation of the Wigner function. Using the operator correspondences for the multimode Wigner function leads to the equation

$$\begin{aligned} \left. \frac{\partial W_{\mathbf{C}}}{\partial t} \right|_{\hat{H}_{\mathbf{C}}} &= \int d^3\mathbf{x} \left\{ \frac{ig}{4\hbar} \frac{\bar{\delta}^2}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x}) \bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} \psi_{\mathbf{C}}^*(\mathbf{x}) \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} + \text{h.c.} \right. \\ &\quad \left. + \frac{i}{\hbar} \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} (H_{\text{sp}} + g [|\psi_{\mathbf{C}}(\mathbf{x})|^2 - \delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x})]) \psi_{\mathbf{C}}(\mathbf{x}) + \text{h.c.} \right\} W_{\mathbf{C}}. \end{aligned} \quad (3.50)$$

The presence of third order derivatives make this equation very difficult to solve. However progress can be made if terms involving these third order derivatives are neglected. We note

that the second functional derivative scales as

$$\frac{\bar{\delta}^2}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})\bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} \sim \frac{1}{|\psi_{\mathbf{C}}(\mathbf{x}, t)|^2} \quad (3.51)$$

which encourages us to neglect the third order derivative terms for appreciable $\mathbf{C}$ -field occupation. This approximation is known as the truncated Wigner approximation, where only derivatives of second order or lower are included [54]. This approximation then gives the equation

$$\left. \frac{\partial W_{\mathbf{C}}}{\partial t} \right|_{\hat{H}_{\mathbf{C}}} = \int d^3\mathbf{x} \left\{ \frac{i}{\hbar} \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} (H_{\text{sp}} + g [|\psi_{\mathbf{C}}(\mathbf{x})|^2 - \delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x})]) \psi_{\mathbf{C}}(\mathbf{x}) + \text{h.c.} \right\} W_{\mathbf{C}}. \quad (3.52)$$

This is a Fokker-Planck equation containing drift terms due to the presence of the first order derivative, but no diffusion due to the absence of second order derivatives. The truncated Wigner approximation is a valid approximation in many cases [12]; in $\mathbf{C}$ -field theory, it is valid when the modes under consideration are significantly occupied. Thus $\mathbf{C}$ -field methods carry the requirement that there is macroscopic occupation in the coherent region such that the truncated Wigner approximation can be made. However, in general, there is a time-scale of validity, after which spurious thermalisation will occur, even if the modes are initially highly occupied [12].

One may map a Fokker-Planck equation to an equivalent stochastic differential equation provided the diffusion matrix is positive semidefinite [55]. This is impossible for the full Wigner function equation of motion due to the presence of the third order derivative terms, as a Fokker-Planck equation contains only first and second order derivatives by definition. Applying the mapping once the truncated Wigner approximation has been made leads to the truncated Wigner projected Gross-Pitaevskii equation

$$i\hbar \frac{\partial \psi_{\mathbf{C}}(\mathbf{x})}{\partial t} = \mathcal{P} \{ (H_{\text{sp}} + g [|\psi_{\mathbf{C}}(\mathbf{x})|^2 - \delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x})]) \psi_{\mathbf{C}}(\mathbf{x}) \}. \quad (3.53)$$

This equation is not explicitly stochastic, however noise is introduced through sampling of the Wigner function for the initial quantum state of the system, resulting in the appropriate half a quantum per mode found in (3.42). The stochastic effects are thus only represented through the initial conditions of the $\mathbf{C}$ -field. The truncated Wigner projected Gross-Pitaevskii equation is not suited to modeling high temperature Bose gases, however it's derivation is important in terms of finding a more suitable theory, the stochastic projected Gross-Pitaevskii equation.

3.5 The Projected Gross-Pitaevskii Equation

The projected Gross-Pitaevskii equation (PGPE) is obtained by applying the projection operator directly to the Heisenberg equation of motion (3.12) [56], and replacing the operator $\hat{\psi}_{\mathbf{C}}$ by a classical field $\psi_{\mathbf{C}}$. This neglects all interactions between the coherent and incoherent regions, and thus the resulting equation of motion includes only the Hamiltonian containing coherent region fields. Again, the mode occupation in the coherent region must be macroscopic. The result is the PGPE

$$i\hbar \frac{\partial \psi_{\mathbf{C}}(\mathbf{x}, t)}{\partial t} = \mathcal{P} \{L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t)\} \quad (3.54)$$

where $L_{\mathbf{C}}$ is the Hamiltonian operator for the $\mathbf{C}$ region

$$L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) = (H_{\text{sp}} + g|\psi_{\mathbf{C}}(\mathbf{x}, t)|^2) \psi_{\mathbf{C}}(\mathbf{x}, t). \quad (3.55)$$

The PGPE may also be formally derived as Hamilton's equation of motion for the $\mathbf{C}$ -field Hamiltonian $H_{\mathbf{C}}$

$$i\hbar \frac{\partial \psi_{\mathbf{C}}(\mathbf{x}, t)}{\partial t} = \frac{\bar{\delta} H_{\mathbf{C}}}{\bar{\delta} \psi_{\mathbf{C}}^*(\mathbf{x}, t)}. \quad (3.56)$$

The PGPE is a microcanonical description of the coherent region, where both the number of particles $N_{\mathbf{C}}$ and the Hamiltonian energy $H_{\mathbf{C}}$ are conserved. There is no dissipative terms in the PGPE and thus any excitations in the coherent region are retained, as are their effect on the coherent region dynamics.

3.6 The Stochastic Projected Gross-Pitaevskii Equation

The formulation of the stochastic projected Gross-Pitaevskii equation (SPGPE) accounts for interactions between the coherent and incoherent regions by treating the incoherent region as being fully thermalised. The incoherent region then acts as a grand canonical reservoir at a specific chemical potential and temperature. All terms from the effective Hamiltonian are included in von Neumann's equation for the density operator, ensuring all interactions are accounted for. One may think of the SPGPE as being an extension of the projected Gross-Pitaevskii equation where extra terms in the final differential equation are included to represent the interactions, with the terms taking the form of extra damping and noise. The full derivation of the SPGPE starting from von Neumann's equation is well documented [1,13]. Here we give a brief outline of the method for deriving the SPGPE.

3.6.1 Master Equation

The evolution of the density operator for the full system is given by the von Neumann equation

$$\partial_t \hat{\rho} = -\frac{i}{\hbar} \left[\hat{H}_{\mathbf{C}} + \hat{H}_{\mathbf{I}} + \hat{H}_{\mathbf{C},\mathbf{I}}, \hat{\rho} \right]. \quad (3.57)$$

The standard procedure for using C-field methods for open systems is to find a master equation for the reduced system, that is the coherent region density operator, by eliminating the degrees of freedom contained within the reservoir [52, 57–60]. This is done by defining the coherent region density operator as the trace of the full system density operator over the incoherent region degrees of freedom

$$\hat{\rho}_{\mathbf{C}} \equiv \text{tr}_{\mathbf{I}} \{ \hat{\rho} \}. \quad (3.58)$$

This is possible as the full system density operator is separable

$$\hat{\rho} = \hat{\rho}_{\mathbf{C}} \otimes \hat{\rho}_{\mathbf{I}} \quad (3.59)$$

as the two sub system density operators $\hat{\rho}_{\mathbf{C}}$ and $\hat{\rho}_{\mathbf{I}}$ are assumed to be uncorrelated.

The tracing procedure results in a number of terms describing interactions between the coherent and incoherent regions. The full master equation for the reduced system is given by

$$\partial_t \hat{\rho}_{\mathbf{C}} = \partial_t \hat{\rho}_{\mathbf{C}}|_H + \partial_t \hat{\rho}_{\mathbf{C}}|_{\gamma} + \partial_t \hat{\rho}_{\mathbf{C}}|_{\varepsilon}. \quad (3.60)$$

The first term $\partial_t \hat{\rho}_{\mathbf{C}}|_H$ originates solely from the Hamiltonian $\hat{H}_{\mathbf{C}}$ involving only the coherent region field operator. The other two terms $\partial_t \hat{\rho}_{\mathbf{C}}|_{\gamma}$ and $\partial_t \hat{\rho}_{\mathbf{C}}|_{\varepsilon}$ arise from the interactions between the coherent and incoherent regions. The terms with the subscripts γ and ε are referred to as number-damping and energy-damping respectively, due to the nature of the processes they represent. The number-damping γ arises from the interaction Hamiltonian terms containing three $\mathbf{I}$ -field operators and one $\mathbf{C}$ -field operator (3.27), while the energy-damping ε arises from the interaction Hamiltonian terms containing two each of the $\mathbf{I}$ -field and $\mathbf{C}$ -field operators (3.28). The nature of these two processes are described later in the chapter. The interaction Hamiltonian terms containing one $\mathbf{I}$ -field operator and three $\mathbf{C}$ -field operators (3.29) do not contribute at this level of approximation [1].

3.6.2 Fokker-Planck Equation

Using the operator correspondences, the full master equation is mapped to an evolution equation for the Wigner function, as was previously done in obtaining the truncated Wigner projected Gross-Pitaevskii equation. This again leads to a partial differential equation with terms containing third order derivatives. As per the truncated Wigner approximation, these

terms are neglected to obtain a valid Fokker-Planck equation

$$\begin{aligned}
\frac{\partial W_{\mathbf{C}}}{\partial t} = & \int d^3\mathbf{x} \left[-\frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} \left(-\frac{i}{\hbar} L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}) + \frac{\gamma}{\hbar} (\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(\mathbf{x}) \right) + \text{h.c.} \right. \\
& \left. + \frac{\gamma k_B T}{\hbar} \frac{\bar{\delta}^2}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x}) \bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x})} + \text{h.c.} \right] W_{\mathbf{C}} \\
& + \int d^3\mathbf{x} \left[-\frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} \left(-\frac{i}{\hbar} V_{\varepsilon}(\mathbf{x}, t) \psi_{\mathbf{C}}(\mathbf{x}) \right) + \text{h.c.} \right. \\
& + \int d^3\mathbf{x}' \frac{k_B T}{\hbar} \varepsilon(\mathbf{x} - \mathbf{x}') \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} \psi_{\mathbf{C}}(\mathbf{x}) \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}^*(\mathbf{x}')} \psi_{\mathbf{C}}^*(\mathbf{x}') + \text{h.c.} \\
& \left. - \int d^3\mathbf{x}' \frac{k_B T}{\hbar} \varepsilon(\mathbf{x} - \mathbf{x}') \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x})} \psi_{\mathbf{C}}(\mathbf{x}) \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(\mathbf{x}')} \psi_{\mathbf{C}}(\mathbf{x}') + \text{h.c.} \right] W_{\mathbf{C}}, \quad (3.61)
\end{aligned}$$

where $L_{\mathbf{C}}$ is the Hamiltonian operator for the $\mathbf{C}$ -field given by (3.55), T and μ are the system temperature and chemical potential respectively, γ is the number-damping rate, $V_{\varepsilon}(\mathbf{x}, t)$ is the scattering potential, and $\varepsilon(\mathbf{x})$ is the scattering amplitude. These last three quantities will be defined in subsection 3.6.4.

Note that second derivatives appear twice in this equation, indicating that there will be more than one noise source in the system. At this point an equivalent stochastic differential equation will help provide a more meaningful interpretation of the various terms.

3.6.3 Stochastic Differential Equation

The mapping of the Fokker-Planck equation to a stochastic differential equation gives the full stochastic projected Gross-Pitaevskii equation

$$(S)d\psi_{\mathbf{C}}(\mathbf{x}, t) = d\psi_{\mathbf{C}}|_H + d\psi_{\mathbf{C}}|_{\gamma} + (S)d\psi_{\mathbf{C}}|_{\varepsilon} \quad (3.62)$$

where

$$d\psi_{\mathbf{C}}|_H = \mathcal{P} \left\{ -\frac{i}{\hbar} L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) dt \right\}, \quad (3.63)$$

$$d\psi_{\mathbf{C}}|_{\gamma} = \mathcal{P} \left\{ \frac{\gamma}{\hbar} (\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(\mathbf{x}, t) dt + dW_{\gamma}(\mathbf{x}, t) \right\}, \quad (3.64)$$

$$(S)d\psi_{\mathbf{C}}|_{\varepsilon} = \mathcal{P} \left\{ -\frac{i}{\hbar} V_{\varepsilon}(\mathbf{x}, t) \psi_{\mathbf{C}}(\mathbf{x}, t) dt + i \psi_{\mathbf{C}}(\mathbf{x}, t) dW_{\varepsilon}(\mathbf{x}, t) \right\}, \quad (3.65)$$

are the Hamiltonian, number-damping, and energy-damping terms respectively, with (S) indicating the stochastic differential equation is in Stratonovich form. The noises $dW_{\gamma}(\mathbf{x}, t)$ and $dW_{\varepsilon}(\mathbf{x}, t)$ will be defined in subsection 3.6.4.

The Hamiltonian term of the SPGPE is simply the PGPE, where there is no consideration of interactions between the coherent and incoherent regions. The latter two terms of (3.62) introduce these interactions.

3.6.4 Energy and Number Damping

The inclusion of interactions between the coherent and incoherent regions lead to dissipative and noise terms which arise physically from number-damping and energy-damping processes. We now give a brief explanation of these processes and the terms describing them.

Number Damping Processes

The second term of the SPGPE corresponds to the increase of particles in the coherent region via the scattering of two thermal particles in the incoherent region, as well as the reverse process; this is shown in Figure 3.2b. Because these are processes through which the coherent region particle number changes, they are referred to as number-damping. They have also been referred to as growth processes, referring to the growth of the coherent region particle number and ultimately the condensate.

The μ and T which appear correspond to the chemical potential and temperature of the thermal reservoir containing the particles in the incoherent region. The number-damping rate γ is in general a function of μ , T and ϵ_{cut} [61]

$$\gamma = \gamma_0 \sum_{j=1}^{\infty} \frac{e^{\beta\mu(j+1)}}{e^{2\beta\epsilon_{\text{cut}}j}} \Phi \left[\frac{e^{\beta\mu}}{e^{2\beta\epsilon_{\text{cut}}}}, 1, j \right]^2 \quad (3.66)$$

where $\beta = 1/k_B T$, $\gamma_0 = 8a_s^2/\lambda_{dB}^2$ with $\lambda_{dB} = \sqrt{2\pi\hbar^2/mk_B T}$ the thermal de Broglie wavelength, and $\Phi[u, v, w]$ the Lerch transcendent.

The noise $dW_{\gamma}(\mathbf{x}, t)$ associated with the number-damping processes is defined by the correlations

$$\langle dW_{\gamma}(\mathbf{x}, t) dW_{\gamma}^*(\mathbf{x}', t) \rangle = \frac{2k_B T}{\hbar} \gamma \delta_{\mathbf{C}}(\mathbf{x}, \mathbf{x}') dt. \quad (3.67)$$

The number-damping noise is complex, additive, and delta correlated in the $\mathbf{C}$ -field.

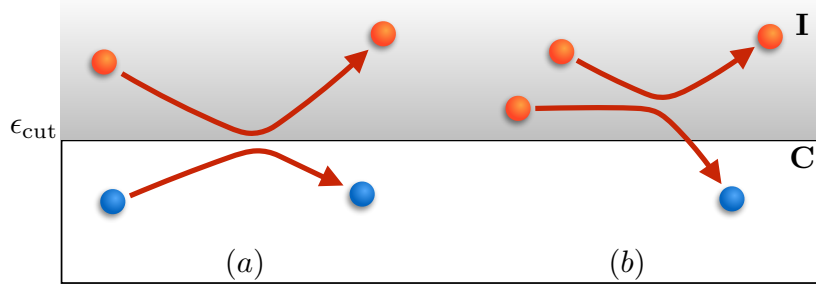


Figure 3.2: A schematic of the two scattering processes that can occur between the **C** and **I** regions. Here blue represents a particle in the **C**-field while orange represents a particle in the **I**-field. The energy-damping process is shown by (a), where a particle in the **C**-field interacts with a particle in the **I**-field, energy is exchanged, and there is no change in particle number of either region. The number-damping process is shown by (b), where two particles in the **I**-field interact, energy is exchanged, and one of the particles moves into the **C**-field.

Energy Damping Processes

The third term of the SPGPE corresponds to the exchange of energy between the coherent and incoherent regions via the scattering of one thermal particle in the incoherent region with one particle in the coherent region, where the outcome of the interaction is one particle in the incoherent region and one in the coherent region; this is shown in Figure 3.2a. The particles can swap regions, but there is no net change in particle number for the respective regions. Thus, this process is number-conserving. Due to the exchange of energy associated with this process and its particle number conserving nature, it is referred to as energy-damping. The energy-damping gives rise to a potential-like term $V_\varepsilon(\mathbf{x}, t)$ in addition to a noise term $dW_\varepsilon(\mathbf{x}, t)$. The energy-damping potential is given by

$$V_\varepsilon(\mathbf{x}, t) = -\hbar \int d^3\mathbf{x}' \varepsilon(\mathbf{x} - \mathbf{x}') \nabla' \cdot \mathbf{j}(\mathbf{x}', t) \quad (3.68)$$

which is dependent on the **C**-field current

$$\mathbf{j}(\mathbf{x}, t) = \frac{i\hbar}{2m} [\psi_{\mathbf{C}}(\mathbf{x}, t) \nabla \psi_{\mathbf{C}}^*(\mathbf{x}, t) - \psi_{\mathbf{C}}^*(\mathbf{x}, t) \nabla \psi_{\mathbf{C}}(\mathbf{x}, t)]. \quad (3.69)$$

The function $\varepsilon(\mathbf{x})$ is defined by

$$\varepsilon(\mathbf{x}) = \frac{\mathcal{M}}{(2\pi)^3} \int d^3\mathbf{k} e^{i\mathbf{k} \cdot \mathbf{x}} S(\mathbf{k}) \quad (3.70)$$

where

$$\mathcal{M} = \frac{16\pi a_s^2}{e^{\beta(\epsilon_{\text{cut}} - \mu)} - 1} \quad (3.71)$$

is the energy-damping rate and $S(\mathbf{k})$ is known as the scattering kernel. The exact form of the scattering kernel depends on the dimensionality of the system. In three dimensions, it is given by

$$S(\mathbf{k}) = \frac{1}{|\mathbf{k}|}. \quad (3.72)$$

The noise $dW_\varepsilon(\mathbf{x}, t)$ associated with the energy-damping process is defined by the correlations

$$\langle dW_\varepsilon(\mathbf{x}, t) dW_\varepsilon(\mathbf{x}', t) \rangle = \frac{2k_B T}{\hbar} \varepsilon(\mathbf{x} - \mathbf{x}') dt. \quad (3.73)$$

The energy-damping noise is real, multiplicative, and has non-local correlations in position space.

3.7 Grand Canonical Equilibrium

The stochastic projected Gross-Pitaevskii equation provides a grand canonical description of the coherent region subject to the chemical potential μ and temperature T of the incoherent region. Regardless of the details of γ , $\mathcal{M}$ or $S(\mathbf{k})$, the SPGPE samples microstates with probability [6]

$$P(\psi_{\mathbf{C}}) \propto \exp\left(\frac{-K_{\mathbf{C}}}{k_B T}\right) \quad (3.74)$$

where the grand canonical Hamiltonian $K_{\mathbf{C}}$ is

$$K_{\mathbf{C}} = H_{\mathbf{C}} - \mu N_{\mathbf{C}} \quad (3.75)$$

and the $\mathbf{C}$ -field Hamiltonian $H_{\mathbf{C}}$ and particle number $N_{\mathbf{C}}$ given by (3.25) and

$$N_{\mathbf{C}} = \int d^3\mathbf{x} |\psi_{\mathbf{C}}(\mathbf{x})|^2 \quad (3.76)$$

respectively.

3.8 Number Damping SPGPE

In situations where there is large amounts of particle transfer between the coherent and incoherent regions, it may be expected that the number-damping processes dominate over the energy-damping processes in determining the system dynamics. With this justification we may ignore the energy-damping terms to obtain the number-damping, or simple growth,

SPGPE

$$d\psi_{\mathbf{C}}(\mathbf{x}, t) = \mathcal{P} \left\{ -\frac{i}{\hbar} L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) dt + \frac{\gamma}{\hbar} (\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(\mathbf{x}, t) dt + dW_{\gamma}(\mathbf{x}, t) \right\}. \quad (3.77)$$

Making this approximation has great benefits in terms of solving the equation of motion numerically, as the presence of additive noise only allows one to use a more efficient algorithm [12]. In fact, the numerical implementation of this equation is only slightly more complicated than for the projected Gross-Pitaevskii equation.

3.8.1 The Damped Projected Gross-Pitaevskii Equation

Neglecting the noise in the number-damping SPGPE gives the damped projected Gross-Pitaevskii equation (DPGPE)

$$i\hbar \frac{\partial \psi_{\mathbf{C}}(\mathbf{x}, t)}{\partial t} = \mathcal{P} \{ L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) + i\gamma (\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(\mathbf{x}, t) \}. \quad (3.78)$$

Evolving with this equation minimises the grand canonical Hamiltonian $K_{\mathbf{C}}$ according to

$$\frac{dK_{\mathbf{C}}}{dt} = -\frac{2\gamma}{\hbar} \int d^3\mathbf{x} |(\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(\mathbf{x}, t)|^2 \quad (3.79)$$

thus damping out all thermal fluctuations, and so the equilibrium solution is the zero temperature PGPE ground state satisfying

$$\mathcal{P} \{ L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) \} = \mu \psi_{\mathbf{C}}(\mathbf{x}, t). \quad (3.80)$$

The coherent region particle number $N_{\mathbf{C}}$ is also damped toward its equilibrium value according to

$$\frac{dN_{\mathbf{C}}}{dt} = -\frac{2\gamma}{\hbar} (\mu(t) - \mu) N_{\mathbf{C}} \quad (3.81)$$

where

$$\mu(t) = \frac{1}{N_{\mathbf{C}}} \int d^3\mathbf{x} \psi_{\mathbf{C}}^*(\mathbf{x}, t) L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) \quad (3.82)$$

is the instantaneous chemical potential.

3.9 Energy Damping SPGPE

We may also conceive of systems where the number-damping process is forbidden, such that the populations of each region is strictly constant. For example, the model could describe a system of one species of particle (the coherent region) in contact with a thermal reservoir

consisting of a different species of particle (the incoherent region). In this case, we ignore the number-damping terms to obtain the energy-damping SPGPE

$$(S)d\psi_{\mathbf{C}}(\mathbf{x}, t) = \mathcal{P} \left\{ -\frac{i}{\hbar} L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) dt - \frac{i}{\hbar} V_{\varepsilon}(\mathbf{x}, t) \psi_{\mathbf{C}}(\mathbf{x}, t) dt + i \psi_{\mathbf{C}}(\mathbf{x}, t) dW_{\varepsilon}(\mathbf{x}, t) \right\}. \quad (3.83)$$

As a consequence of the multiplicative noise, the numerical implementation of this equation requires different algorithms to the number-damping case. Unfortunately the algorithm required can be numerically intensive¹, and this can hold back exploration of systems described by this equation.

Ignoring the noise gives an energy-damping equivalent to the DPGPE

$$(S)d\psi_{\mathbf{C}}(\mathbf{x}, t) = \mathcal{P} \left\{ -\frac{i}{\hbar} L_{\mathbf{C}} \psi_{\mathbf{C}}(\mathbf{x}, t) dt - \frac{i}{\hbar} V_{\varepsilon}(\mathbf{x}, t) \psi_{\mathbf{C}}(\mathbf{x}, t) dt \right\}. \quad (3.84)$$

Evolving with this equation minimises the grand canonical Hamiltonian $K_{\mathbf{C}}$ according to

$$\frac{dK_{\mathbf{C}}}{dt} = -\hbar \mathcal{M} \int d^3 \mathbf{k} S(\mathbf{k}) |\mathbf{k} \cdot \mathbf{j}(\mathbf{k}, t)|^2 \quad (3.85)$$

where $\mathbf{j}(\mathbf{k}, t)$ is the Fourier transform of the $\mathbf{C}$ -field current. It can be shown from the SPGPE that neglecting number-damping terms gives the coherent region particle number evolution

$$\frac{dN_{\mathbf{C}}}{dt} = 0, \quad (3.86)$$

consistent with the number-conserving nature of the energy-damping process.

3.10 Reduced Dimensionality

Solving the full three-dimensional SPGPE is generally a numerically challenging task. However experiments in Bose-condensed systems are often conducted in regimes where part of the system can be considered to be either quasi-one-dimensional or quasi-two-dimensional. For example, a partially condensed Bose gas strongly confined to a toroid may be considered a one dimensional superfluid in contact with a three dimensional thermal cloud. In this section we will consider the modelling of a system that is quasi-one-dimensional due to the presence of strong harmonic confinement along the transverse dimensions. A full account of the dimensional reduction procedure is presented in [62], here we simply present an outline of the derivation.

¹See subsection 4.5.3 for further discussion

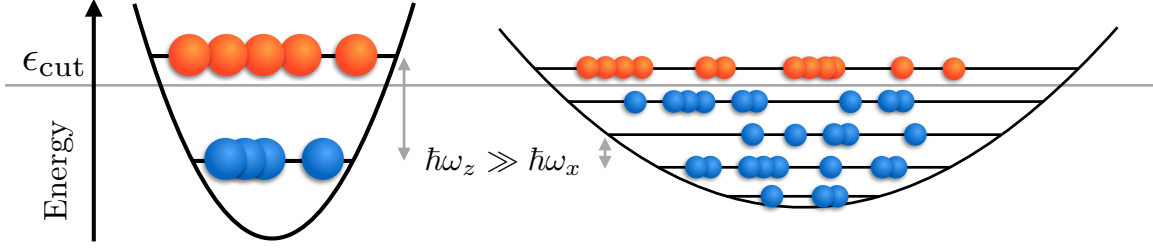


Figure 3.3: A schematic of the low-dimensional system. The blue represents the **C**-field while orange represents the **I**-field. In the subspace of the strongly confined dimensions (here we show the z dimension) the imposed energy cut-off allows only the lowest energy state in the **C**-field, while multiple energy states are accessible in the x dimension subspace.

3.10.1 Reduction Procedure

The system is assumed to be confined in the potential

$$V(\mathbf{x}) = \frac{1}{2}m\omega_{\perp}^2(y^2 + z^2) + V(x) \quad (3.87)$$

where $V(x)$ is any trapping potential in the x dimension. If the energy of the transverse ground state is comparable to the thermal energy

$$\hbar\omega_{\perp} \lesssim k_B T \quad (3.88)$$

then it will be a good approximation to introduce the energy cutoff for the transverse modes as $\epsilon_{\text{cut}} \sim \hbar\omega_{\perp}/2$, such that only the lowest energy transverse mode is contained in the **C**-field. All higher energy modes become part of the **I**-field, as is demonstrated in Figure 3.3.

In the tightly confined dimensions we then assume separability and the ground state wave functions

$$\phi_0(y) = \left(\frac{\eta}{\pi}\right)^{1/2} e^{-\eta y^2/2}, \quad \phi_0(z) = \left(\frac{\eta}{\pi}\right)^{1/2} e^{-\eta z^2/2} \quad (3.89)$$

where

$$\eta = \frac{m\omega_{\perp}}{\hbar} = \frac{1}{a_{\perp}^2} \quad (3.90)$$

with $a_{\perp}$ the transverse oscillator length. Projecting out the transverse dimensions to obtain an effective one dimensional equation of motion is then defined by the operation

$$\mathcal{P}_{\perp} \{F(\mathbf{x})\} \equiv \int dy \int dz |\phi_0(y)|^2 |\phi_0(z)|^2 F(\mathbf{x}) = F(x) \quad (3.91)$$

where the dimensionality of any function is denoted by its spatial argument with $\mathbf{x}$, $\mathbf{x}_{\perp}$, and x corresponding to three dimensions, two dimensions, and one dimension respectively. This

projection is applied to every term in the stochastic projected Gross-Pitaevskii equation to obtain its form in one dimension. The only other consideration needed is for the noise terms, where a double projection of the correlations is more convenient than projecting the noise directly

$$\begin{aligned} \langle dW(x, t) dW^*(x', t) \rangle &= \int dy \int dz |\phi_0(y)|^2 |\phi_0(z)|^2 \\ &\times \int dy' \int dz' |\phi_0(y')|^2 |\phi_0(z')|^2 \langle dW(\mathbf{x}, t) dW^*(\mathbf{x}', t) \rangle. \end{aligned} \quad (3.92)$$

The results of these projections are presented in the following subsection.

3.10.2 One Dimensional Stochastic Projected Gross-Pitaevskii Equation

Projecting out the transverse dimensions gives the one dimensional stochastic projected Gross-Pitaevskii equation

$$(S)d\psi_{\mathbf{C}}(x, t) = d\psi_{\mathbf{C}}|_H + d\psi_{\mathbf{C}}|_{\gamma} + (S)d\psi_{\mathbf{C}}|_{\varepsilon} \quad (3.93)$$

where

$$d\psi_{\mathbf{C}}|_H = \mathcal{P} \left\{ -\frac{i}{\hbar} L_{\mathbf{C}} \psi_{\mathbf{C}}(x, t) dt \right\}, \quad (3.94)$$

$$d\psi_{\mathbf{C}}|_{\gamma} = \mathcal{P} \left\{ \frac{\gamma}{\hbar} (\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(\mathbf{x}, t) dt + dW_{\gamma}(x, t) \right\}, \quad (3.95)$$

$$(S)d\psi_{\mathbf{C}}|_{\varepsilon} = \mathcal{P} \left\{ -\frac{i}{\hbar} V_{\varepsilon}(x, t) \psi_{\mathbf{C}}(x, t) dt + i\psi_{\mathbf{C}}(x, t) dW_{\varepsilon}(x, t) \right\}. \quad (3.96)$$

Now $L_{\mathbf{C}}$ is the one dimensional Hamiltonian operator for the $\mathbf{C}$ -field

$$L_{\mathbf{C}} \psi_{\mathbf{C}}(x, t) = (H_{\text{sp}} + g_1 |\psi_{\mathbf{C}}(x, t)|^2) \psi_{\mathbf{C}}(x, t) \quad (3.97)$$

with H_{sp} the one dimensional single particle Hamiltonian of the form

$$H_{\text{sp}} = -\frac{\hbar^2}{2m} \partial_{xx} + V(x) \quad (3.98)$$

and $g_1 = 2\hbar\omega_{\perp} a_s$ the one dimensional interaction parameter. The energy-damping potential

is given in one dimension by

$$V_\varepsilon(x, t) = -\hbar \int dx' \varepsilon(x - x') \partial_{x'} j(x', t) \quad (3.99)$$

where $j(x, t)$ is the one dimensional **C**-field current

$$j(x, t) = \frac{i\hbar}{2m} [\psi_{\mathbf{C}}(x, t) \partial_x \psi_{\mathbf{C}}^*(x, t) - \psi_{\mathbf{C}}^*(x, t) \partial_x \psi_{\mathbf{C}}(x, t)] \quad (3.100)$$

and the function $\varepsilon(x)$ is defined as

$$\varepsilon(x) = \frac{\mathcal{M}}{2\pi} \int dk e^{ikx} S_1(k). \quad (3.101)$$

As mentioned earlier, the form of the scattering kernel depends on the dimensionality of the system. The one dimensional scattering kernel is

$$S_1(k) = \sqrt{\frac{\eta}{8\pi}} G\left(\frac{|k|}{\sqrt{2\eta}}\right) \quad (3.102)$$

with $G(x) = \exp(x^2) \operatorname{erfc}(x)$ the scaled complementary error function.

The one dimensional number-damping noise has the correlation

$$\langle dW_\gamma(x, t) dW_\gamma^*(x', t) \rangle = \frac{2k_B T}{\hbar} \gamma \delta_{\mathbf{C}}(x, x') dt \quad (3.103)$$

while the one dimensional energy-damping noise has the correlation

$$\langle dW_\varepsilon(x, t) dW_\varepsilon(x', t) \rangle = \frac{2k_B T}{\hbar} \varepsilon(x - x') dt. \quad (3.104)$$

We use the one dimensional stochastic Gross-Pitaevskii equation throughout this work. We will use the number-damping one-dimensional SPGPE, the energy-damping one dimensional SPGPE, and the full one dimensional SPGPE as appropriate.

The regime of validity for the one-dimensional SPGPE used in this thesis has been studied [62]. Qualitatively, the regime of validity for a system consisting of a single component is rather small, as confining the system tighter can result in the thermal cloud losing its three-dimensional nature. In contrast the regime of validity for a system of two components is fairly large, as the thermal component can be trapped separately. In this work we treat the one-dimensional SPGPE as a model, under the assumption that **C**-field is one-dimensional in nature, while the thermal **I**-field retains three-dimensional characteristics.

3.11 Numerical Methods

Solving any form of the SPGPE is a non-trivial task, which many researchers have dedicated time to. In this work, we use an adaptive Runge-Kutta method in the interaction picture to solve the number-damping SPGPE numerically [63, 64]. The presence of multiplicative noise in the full and energy-damping SPGPE render this method insufficient; for these equations a semi-implicit Euler method is used [7, 65]. The downside of this is that the semi-implicit Euler method is significantly more time-consuming than the adaptive Runge-Kutta method, with hefty computational resources required to make implementation feasible for three dimensional systems. Since we are working with one dimensional systems, implementation of this method can be done in reasonable time frames. Some further discussion on numerical solutions of the SPGPE may be found in subsection 4.5.3 while detailed discussions may be found elsewhere [7, 63–65].

Chapter 4

The Kibble-Zurek Mechanism

4.1 Introduction

The origins of the Kibble-Zurek mechanism (KZM) are relatively recent, with the first of two papers by Kibble on domain structure in the early universe published in 1976 [44], and the first application of the idea by Zurek to topological defects in condensed matter systems published in 1985 [46]. Kibble based his analysis on equilibrium statistical mechanics, while Zurek introduced a theory of transitions occurring in a finite time. Despite the relatively short time frame since its inception, the field has matured to the point where it has generally been confirmed that topological defects do form via KZM in a variety of systems [5, 66–74], although some exceptions do exist [75]. The key testable consequence of KZM is the scaling of the density of defects with the quench rate. The surprising prediction of KZM is that this scaling is dependent on the equilibrium critical exponents of the system under consideration, that is, a non-equilibrium effect is predicted using equilibrium properties, due to the universal dynamics of critical phenomena near the transition [46, 47].

Experiments testing the KZM hypothesis generally involve forcing the system across a second order phase transition by quenching some external parameter and measuring the number of defects that form. There are several complications that can arise with this procedure. The defects produced may be unstable, forcing one to instead measure some remnant of post-quench dissipative evolution that may scale less favourably with quench rate. The relationship between defect density and quench rate is generally a power law, and the exponent tends to be significantly less than one. Thus to obtain significant variations in the defect density the quench rate must be varied over a large range. Furthermore, actually performing a linear quench can be a difficult task. A common parameter to quench is the temperature, and the resultant temperature gradients in the system can suppress defect formation [76, 77] and also drive convection that creates defects, but not via the KZM [75, 78].

Bose-Einstein condensates (BECs) in dilute alkali gases provide a useful platform for experimental tests of KZM. Bose-Einstein condensation is a second order phase transition that

can be crossed by changing the system temperature, but also by changing the system chemical potential. In numerical studies, the transition is generally induced by varying the chemical potential [50,79]. In practice most experiments also use this method, with the quench effected by evaporative cooling that induces relatively small changes in absolute temperature combined with significant changes in particle number. There have been a number of experiments testing KZM in BECs. Temperature quenches resulted in defects being produced as predicted by KZM in [5,73], with [73] obtaining a power law agreeing with mean-field theory. A test on the power-law of persistent currents after a temperature quench [74] also showed agreement with mean-field theory. However a more recent experiment [80] involving measurement of correlation lengths did not agree with mean-field theory, but instead favoured the predictions of the F-model [81], a model for superfluid helium utilising pseudospins. The discrepancy of results between different experiments shows that there is still much work to be done on this problem.

In this chapter we present the relevant derivations of the equations of KZM. The initial equations are for the density of topological defects, which can generally be applied to any system. We also derive equations for the scaling of winding numbers in toroidally trapped superfluids. We then present our results of simulating the quench of a toroidally trapped Bose gas across the Bose-Einstein condensation transition, numerically solving both the full stochastic projected Gross-Pitaevskii equation and its sub theory, the number-damping stochastic projected Gross-Pitaevskii equation. Our aim is to test the concepts of KZM against a rigorous (although approximate) theory that includes higher order reservoir interactions.

4.2 General Formulation

Consider a system undergoing spontaneous symmetry breaking induced by the change of a parameter λ . The second order phase transition occurs when the parameter reaches a critical point λ_c , and the quench across the transition involves λ approaching λ_c from above. It is convenient to define the *reduced distance parameter*

$$\varepsilon = \frac{\lambda_c - \lambda}{\lambda_c} \quad (4.1)$$

such that the system is in the symmetric phase for $\varepsilon < 0$, the asymmetric phase for $\varepsilon > 0$, and the transition occurs at $\varepsilon = 0$. A characterisation of second order phase transitions is the divergence of both the equilibrium correlation length

$$\xi(\varepsilon) = \frac{\xi_0}{|\varepsilon|^\nu} \quad (4.2)$$

and the equilibrium relaxation time

$$\tau(\varepsilon) = \frac{\tau_0}{|\varepsilon|^{z\nu}} \quad (4.3)$$

as the transition point is approached, where ξ_0 and τ_0 are constants that depend on the microscopic details of the system [16]. Here we have introduced the correlation length critical exponent ν and the dynamic critical exponent z , that by convention is expressed in terms of ν , as given in the form (4.3). In contrast to the constants ξ_0 and τ_0 , the critical exponents ν and z do not depend on the microscopic details of the system, but instead are determined by the universality class of the transition [16]. For any quench protocol we can usually linearise the time-dependent $\lambda(t)$ around the critical point λ_c . Thus we assume the case of a linear quench

$$\lambda(t) = \lambda_c [1 - \varepsilon(t)] \quad (4.4)$$

which is symmetric around the critical point. The quench is characterised by the quench rate τ_Q such that the reduced parameter varies linearly in time as

$$\varepsilon(t) = \frac{t}{\tau_Q} \quad (4.5)$$

and the critical point is reached at $t = 0$. If we quench the reduced parameter from $-\varepsilon_0$ to ε_0 then the time over which the quench is performed is $t \in [-\varepsilon_0\tau_Q, \varepsilon_0\tau_Q]$.

When the parameter is far from the critical point $|\lambda| \gg \lambda_c$, the equilibrium relaxation time is very small compared to the time remaining before the critical point is reached. Thus at this stage of the quench, the dynamics are essentially adiabatic and the system follows the instantaneous equilibrium state. As the critical point is approached, the equilibrium relaxation time increases until it is equal to the time remaining before the critical point is reached. At this point, the system can no longer respond adiabatically to the changing parameter and the dynamics become approximately frozen. Thus this point is referred to as the freeze-out time. Once this point is reached on the other side of the transition, the system returns to following the changing parameter adiabatically. The theory of KZM thus splits the system dynamics into three stages where the dynamics are adiabatic, then effectively frozen, then adiabatic once more. This simplification is referred to as the adiabatic-impulse approximation, with the frozen dynamics stage being referred to as the impulse regime.

During the quench, the correlation length will also be changing according to (4.2) until the freeze-out time is reached. At this point the correlation length is frozen while the system passes through the impulse regime. This freeze-out correlation length will determine the size of the domains that form as the system undergoes the phase transition. At the phase transition, there is local breaking of symmetry throughout the system, and hence each domain is assigned

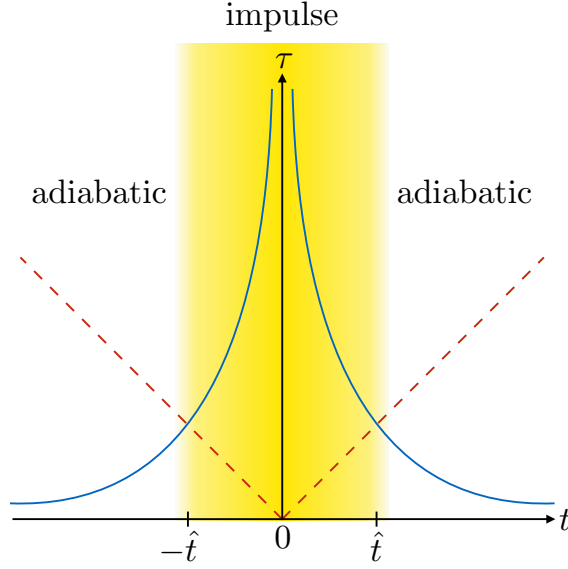


Figure 4.1: A schematic demonstrating the adiabatic-impulse approximation in the Kibble-Zurek scenario. The solid blue line represents the instantaneous relaxation time, while the dashed red line represents the time remaining until the transition ($t < 0$), or the time passed since the transition ($t > 0$), where the transition occurs at $t = 0$. Where the two lines intersect defines the *freeze-out time* $\hat{t}$ and the *impulse regime* $t \in [-\hat{t}, \hat{t}]$. Here the impulse regime is shown in yellow.

a random phase independent of the surrounding domains. Once the system is released from the impulse regime, the domains that have formed will merge and topological defects will form where the phases of the domains are not the same. Thus the number of topological defects in the system is determined by the freeze-out correlation length, which is determined by the freeze-out time, which is determined by the quench rate.

The freeze-out time $\hat{t}$ is found by equating the time remaining until the transition is reached with the equilibrium relaxation time

$$\tau(\varepsilon(\hat{t})) = \hat{t}, \quad (4.6)$$

such that there is only just enough time for the system to come to equilibrium; this is demonstrated in Figure 4.1. This freeze-out time is thus given by [46]

$$\hat{t} = (\tau_0 \tau_Q^{z\nu})^{\frac{1}{1+z\nu}} \propto \tau_Q^\alpha, \quad (4.7)$$

where

$$\alpha \equiv \frac{z\nu}{1+z\nu} \quad (4.8)$$

and the freeze-out value of the reduced parameter is then

$$\hat{\varepsilon} \equiv |\varepsilon(\hat{t})| = \left(\frac{\tau_0}{\tau_Q} \right)^{\frac{1}{1+z\nu}} \quad (4.9)$$

where we have used (4.2) and (4.3). The average size of the domains formed during the transition is given by the equilibrium correlation length at the freeze-out time

$$\hat{\xi} \equiv \xi(\hat{\varepsilon}) = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{\nu}{1+z\nu}} \quad (4.10)$$

which also sets the average distance between the topological defects formed after the domains merge. This scaling of the correlation length with τ_Q is the key prediction of KZM.

Power laws are obtained for these quantities only because the relaxation time scales as a power law of the reduced parameter. However this may not always be the case; for example the Kosterlitz-Thouless transition has a relaxation time with an exponential dependence on ε resulting in a more complex dependence of $\hat{t}$ and $\hat{\xi}$ on τ_Q [82].

The prediction (4.10) is generally rewritten to predict the density of topological defects [16]

$$n \approx \frac{\hat{\xi}^d}{\hat{\xi}_D^d} = \frac{1}{\xi_0^{D-d}} \left(\frac{\tau_0}{\tau_Q} \right)^{(D-d)\frac{\nu}{1+z\nu}} \quad (4.11)$$

where D and d are the dimensions of the system and the defects respectively (e.g. $D = 2$ and $d = 0$ for vortices in a 2D superfluid). This equation tends to overestimate the actual density of defects that is observed in numerics, so a dimensionless factor f is often introduced such that $\hat{\xi}$ is replaced by $f\hat{\xi}$, where $f \sim \mathcal{O}(1 - 10)$ with the actual value dependent on the model [49, 79, 83, 84]. Thus the result is that KZM gives an estimate for the order of magnitude of the density of defects rather than an exact prediction. Regardless of this, one needs only to check the power law scaling to claim that KZM holds and show that the dynamics across the phase transition are indeed universal. One thus requires the ability to measure the number of defects after a quench, and to repeat this for a large range of quench times.

4.2.1 Fast Quench Limit

The time over which the quench takes place is dependent on both the quench rate τ_Q and the initial (and final) values of the reduced distance parameter ε_0 . We define the ramp time as being the time between the start of the quench and the transition

$$t_r = \varepsilon_0 \tau_Q \quad (4.12)$$

such that the entire quench takes place over $2t_r$. If we inspect (4.7) we see that one may be able to set a quench rate such that the freeze-out time is greater than the ramp time. This

is of course entirely unphysical as it would require the system to freeze at the correct time before the quench has even started, somehow having prior knowledge of what the quench rate will be. Thus we can be sure that the predictions of KZM can only hold if the freeze-out time is less than the ramp time $\hat{t} < t_r$. We can define the timescale

$$\tau_m = \tau_0 \varepsilon_0^{-(1+z\nu)} \quad (4.13)$$

such that for $\tau_Q < \tau_m$ the system is in the fast quench limit. If the parameter is quenched at a rate faster than τ_m^{-1} then the system will no longer follow the quench, but will instead respond as if it was an instantaneous change. In fact we may expect the scaling to break down even as we approach the fast-quench limit, as the total time spent frozen becomes comparable to the total quench time.

4.3 Winding Numbers in Loops

We are primarily interested in the Bose-Einstein condensation transition in a one dimensional Bose gas. In such a system, the defects that form as a result of merging domains are dark solitons [73]. However the problem arises that dark solitons are only stable at zero temperature [41, 50, 85, 86], which is not generally the case, and thus after a quench the newly formed dark solitons will decay relatively quickly. Even if one does have the ability to measure the number of solitons at some point before they have all decayed, it is not clear at what time the number should even be measured to allow valid comparisons between quench rates. If one insists on measuring the number of solitons to verify (or otherwise) KZM, then the soliton number would have to be continuously measured such that the function giving the soliton number with respect to time could be shown to have a universal rescaling, as is done in [50]. This route also suffers from the problem of distinguishing between solitons and density fluctuations due to noise during early growth of the condensate.

Fortunately there is an alternative to soliton counting available if the system has periodic boundary conditions, such as when the Bose gas is confined in a toroidal trap. After the domains have merged and the resultant solitons have decayed away, the new equilibrium state may contain a non-zero winding. The winding is topologically stable [87] and thus can be accurately measured post-quench, with the only restriction being the system lifetime itself. The statistics of the final winding can be obtained to test the KZM theory [46, 79].

Consider a one dimensional Bose gas confined in a toroid of circumference L . At the freeze-out time the typical domain size is given by (4.10) and thus the number of independent phase domains in the gas is

$$N \approx \frac{L}{\hat{\xi}}. \quad (4.14)$$

The probability density for the phase of any one domain is uniform between $-\pi$ and π and can be represented functionally by

$$P(\theta) = \frac{1}{2\pi} \Pi\left(\frac{\theta}{2\pi}\right) \quad (4.15)$$

where $\Pi(t)$ is the rectangular function defined by

$$\Pi(t) = \begin{cases} 0 & \text{if } |t| > \frac{1}{2} \\ 1 & \text{if } |t| \leq \frac{1}{2}. \end{cases} \quad (4.16)$$

The variance of the phase is thus

$$\sigma^2(\theta) = \int_{-\infty}^{\infty} d\theta \theta^2 P(\theta) = \int_{-\pi}^{\pi} d\theta \frac{\theta^2}{2\pi} = \frac{\pi^2}{3}. \quad (4.17)$$

The variance of the phase difference between two neighbouring domains is then

$$\sigma^2(\Delta\theta_i) = \sigma^2(\theta_{i+1} - \theta_i) = \sigma^2(\theta_{i+1}) + \sigma^2(\theta_i) = \frac{2\pi^2}{3} \quad (4.18)$$

and so the variance of the accumulated phase around the toroid is

$$\sigma^2(\theta_c) = \sum_{i=1}^{N-1} \sigma^2(\Delta\theta_i) = (N-1) \frac{2\pi^2}{3} \approx N \frac{2\pi^2}{3} \approx \frac{L}{\hat{\xi}} \frac{2\pi^2}{3} \quad (4.19)$$

where we have assumed that N is appreciably greater than one. This amounts to assuming that the typical domain size $\hat{\xi}$ is not comparable to the system size L . If this is not the case then the scaling law can be different [74], but we do not consider this case further in this work. The winding number of the system is related to the accumulated phase by

$$\mathcal{W} = \frac{\theta_c}{2\pi} \quad (4.20)$$

and thus the variance of the winding is given by

$$\sigma^2(\mathcal{W}) = \frac{1}{(2\pi)^2} \sigma^2(\theta_c) \approx \frac{1}{6} \frac{L}{\hat{\xi}}. \quad (4.21)$$

According to KZM, the standard deviation of the winding after the system has reached a post-quench equilibrium is then given by, using (4.10) and (4.21),

$$\sigma(\mathcal{W}) = \sqrt{\frac{L}{6\hat{\xi}_0}} \tau_0^{\frac{\nu}{2(1+z\nu)}} \tau_Q^{\frac{-\nu}{2(1+z\nu)}} \propto \tau_Q^{-\beta} \quad (4.22)$$

where

$$\beta \equiv \frac{\nu}{2(1+z\nu)}. \quad (4.23)$$

Following a quench, the system may be left to return to a stable state which may contain some non-zero winding. This winding can then be measured experimentally by interferometry [74, 88] or other methods. Experimental temperature quenches have been performed in toroidally trapped BECs [74] where the power-law exponents agreed with mean-field theory. The downside to measuring the winding over the defects themselves is that it is a distribution, and thus more trajectories must be run to obtain good statistics. Furthermore, the power-law exponent for the winding is half that for defects, requiring greater experimental control for testing.

4.4 Correlations of the SPGPE

The formulation of the KZM equations required the equilibrium correlation length and relaxation time of the system under consideration, and their dependence on the reduced distance parameter. If there exists an analytic model that describes the evolution of the system, then one can in principle extract the equilibrium correlation length and relaxation time as functions of the quenched parameter. This will also reveal the critical exponents ν and z by comparison with (4.10) and (4.3), provided the functions are indeed power laws, which is not guaranteed [82]. Extraction of the equilibrium correlation length and relaxation time can be done by finding the equal-time and equal-space correlation functions of the system, and identifying the characteristic length or time scales over which they decay.

The model we are considering is the stochastic projected Gross-Pitaevskii equation (SPGPE) (3.93). The parameter we wish to vary is the chemical potential μ , with the Bose-Einstein condensation transition occurring at $\mu_c = 0$. The quench we are considering is then defined by

$$\mu(t) = \frac{t}{\tau_Q} E_0 \quad (4.24)$$

where E_0 is a characteristic energy scale of the system, and we quench from $-\mu_0$ to μ_0 . The time over which the quench takes places is thus $t \in [-\tau_Q \mu_0 / E_0, \tau_Q \mu_0 / E_0]$. The critical value being zero is not compatible with the original definition of the reduced distance parameter (4.1), and so we propose an alternative definition to accommodate this

$$\epsilon(t) = \frac{\mu(t)}{E_0}, \quad (4.25)$$

which, with (4.24), gives the linear quench (4.5). For the characteristic energy scale we use

the transverse harmonic trapping energy

$$E_0 = \hbar\omega_\perp \quad (4.26)$$

where $\omega_\perp$ is the transverse trapping frequency.

Although finding any sort of analytic solutions to the full SPGPE, even in one dimension, is very difficult, some analytic progress can be made for the number-damping sub theory, given in one dimension by

$$d\psi_{\mathbf{C}}(x, t) = \mathcal{P} \left\{ \frac{1}{\hbar} (i + \gamma) (\mu - L_{\mathbf{C}}) \psi_{\mathbf{C}}(x, t) dt + dW_\gamma(x, t) \right\}. \quad (4.27)$$

Here $L_{\mathbf{C}}$ is the Gross-Pitaevskii Hamiltonian

$$L_{\mathbf{C}}\psi_{\mathbf{C}}(x, t) = \left(-\frac{\hbar^2}{2m} \partial_{xx} + g_1 |\psi_{\mathbf{C}}(x, t)|^2 \right) \psi_{\mathbf{C}}(x, t) \quad (4.28)$$

where γ is the number-damping rate, $dW_\gamma(x, t)$ is the number-damping noise, and g_1 is the one dimensional interaction strength, related to the s-wave scattering length a_s and transverse harmonic trapping frequency $\omega_\perp$ by

$$g_1 = 2\hbar\omega_\perp a_s. \quad (4.29)$$

The number-damping noise has the correlation

$$\langle dW_\gamma(x, t) dW_\gamma^*(x', t) \rangle = \frac{2k_B T}{\hbar} \gamma \delta_{\mathbf{C}}(x, x'). \quad (4.30)$$

If we are on the symmetric side of the transition ($\mu < 0$), then we may make the approximation

$$g_1 |\psi_{\mathbf{C}}(x, t)|^2 \approx 0, \quad (4.31)$$

since the number density will be very low. Making this approximation allows us to transform (4.27) into momentum space. This gives the equation of motion

$$\hbar d\phi(k, t) = (i + \gamma) \left(\mu - \frac{\hbar^2 k^2}{2m} \right) \phi(k, t) dt + \hbar dU_\gamma(k, t) \quad (4.32)$$

where

$$\phi(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \psi_{\mathbf{C}}(x, t) \quad (4.33)$$

is the $\mathbf{C}$ -field wave function in momentum space and

$$dU_\gamma(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} dW_\gamma(x, t) \quad (4.34)$$

is the number-damping noise in momentum space. The general solution to (4.32) is then given by

$$\phi(k, t) = e^{-\int_0^t dt' \Lambda(k, t')} \phi(k, 0) + \int_0^t dt' e^{-\int_t^{t'} ds \Lambda(k, s)} dU(k, t') \quad (4.35)$$

where

$$\hbar \Lambda(k, t) = (i + \gamma) \left(\frac{\hbar^2 k^2}{2m} - \mu \right). \quad (4.36)$$

4.4.1 Steady State

In order to obtain the equilibrium values of the correlation length and relaxation time, in the form of (4.40) and (4.3), we need to consider the steady state correlations of the system. Thus we find the correlations for a constant chemical potential. Since we have already assumed that we are on the symmetric side of the phase transition, the chemical potential is negative. The coefficient (4.36) is now time-independent, making the integrals in (4.35) trivial. Taking $\langle \phi^*(k, t) \phi(k', t') \rangle$ from (4.35) and letting $t, t' \rightarrow 0$, while keeping $|t - t'|$ constant and finite, we then transform back to position space to obtain the steady state correlation function

$$\langle \psi_{\mathbf{C}}^*(x, t) \psi_{\mathbf{C}}(x', t') \rangle = \frac{k_B T}{2\pi|\mu|} I(x - x') e^{-(\gamma+i)\frac{|\mu|}{\hbar}|t-t'|} \quad (4.37)$$

where

$$I(x) = \int_{-\infty}^{\infty} dk e^{ikx} \frac{\exp \left\{ -(\gamma + i) \frac{\hbar k^2}{2m} |t - t'| \right\}}{1 + \hbar^2 k^2 / 2m|\mu|}. \quad (4.38)$$

To obtain the equal-time correlation function we set $t = t'$. The correlation function then simplifies to

$$\langle \psi_{\mathbf{C}}^*(x, t) \psi_{\mathbf{C}}(x', t) \rangle = \frac{k_B T}{2|\mu|\xi} e^{-|x-x'|/\xi} \quad (4.39)$$

where we have identified the equilibrium correlation length

$$\xi \equiv \sqrt{\frac{\hbar^2}{2m|\mu|}}. \quad (4.40)$$

If we instead set $x = x'$ and assume $|\mu||t - t'|/\hbar$ is large, then we obtain the equal-position correlation function

$$\langle \psi_{\mathbf{C}}^*(x, t) \psi_{\mathbf{C}}(x, t') \rangle = \frac{k_B T}{2|\mu|\xi} \frac{e^{-(1+i/\gamma)|t-t'|/\tau}}{\sqrt{\pi(1+i/\gamma)|t-t'|/\tau}} \quad (4.41)$$

where we have identified the equilibrium relaxation time

$$\tau \equiv \frac{\hbar}{\gamma|\mu|}. \quad (4.42)$$

Comparing (4.40) and (4.42) with (4.2) and (4.3) we can identify the constants

$$\xi_0 = \frac{\hbar}{\sqrt{2mE_0}}, \quad (4.43)$$

$$\tau_0 = \frac{\hbar}{\gamma E_0}, \quad (4.44)$$

in addition to the critical exponents $\nu = 1/2$ and $z = 2$. These are the critical exponents predicted by mean-field theory.

4.4.2 Linear Quench

Here we consider the correlations for a linear quench of the chemical potential of the form (4.24), as in done in [50]. The coefficient (4.36) is now time-dependent, which increases the complexity of the problem. To allow some analytic progress to be made, we simplify by only concerning ourselves with the equal-time correlations and so set $t = t'$, as well as making the approximation that the initial chemical potential μ_0 is very large. Integrating (4.35) and transforming the correlation of the solution to position space, we find the time-dependent correlation function

$$\langle \psi_{\mathbf{C}}^*(x, t) \psi_{\mathbf{C}}(x', t) \rangle = \frac{k_B T}{2|\hat{\mu}|\hat{\xi}} f\left(\frac{|x - x'|}{\hat{\xi}}, \frac{\hat{\xi}}{\xi(t)}\right) \quad (4.45)$$

where

$$f(x, y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dk e^{ikx} G(k^2 + y^2) \quad (4.46)$$

with $G(x) \equiv e^{x^2} \operatorname{erfc}(x)$ the scaled complementary error function and we have identified the freeze-out correlation length

$$\hat{\xi} = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{\nu}{1+z\nu}} = \frac{\hbar}{\sqrt{2m}} \left(\frac{\gamma\tau_Q}{\hbar E_0} \right)^{\frac{1}{4}} \quad (4.47)$$

and freeze-out chemical potential

$$\hat{\mu} = \left(\frac{\tau_0}{\tau_Q} \right)^{\frac{1}{1+z\nu}} = \left(\frac{\hbar E_0}{\gamma\tau_Q} \right)^{\frac{1}{2}}. \quad (4.48)$$

We note that all the spatial dependence of (4.49) is through the quantity $x - x'$, thus we may rewrite it as a function of the single variable $r = x - x'$

$$\rho(r, t) \equiv \langle \psi_{\mathbf{C}}^*(x, \hat{t}) \psi_{\mathbf{C}}(x', \hat{t}) \rangle = \frac{k_B T}{2|\hat{\mu}|\hat{\xi}} f \left(\frac{|r|}{\hat{\xi}}, \frac{\hat{\xi}}{\xi(t)} \right). \quad (4.49)$$

We may also refer to the quantity $\rho(r, t)$ as the *one body density matrix*. The result (4.49) is similar to that found in [50], although we have derived the correlation function for a slightly different equation. Of interest is the correlation function at the freeze-out time. Setting $t = \hat{t}$ in (4.49) results in the slightly simpler expression

$$\rho(r, \hat{t}) \equiv \langle \psi_{\mathbf{C}}^*(x, \hat{t}) \psi_{\mathbf{C}}(x', \hat{t}) \rangle = \frac{k_B T}{2|\hat{\mu}|\hat{\xi}} f \left(\frac{|r|}{\hat{\xi}}, 1 \right). \quad (4.50)$$

We have thus obtained a universal form of the correlation function at the freeze-out time where there is only one length scale present, the freeze-out correlation length $\hat{\xi}$.

4.5 Numerical Procedure

We simulate quenches of chemical potential across the Bose-Einstein condensation transition for a one dimensional toroidally trapped Bose gas and compare the results to those predicted by KZM and mean-field theory. These are simulated by numerically solving either the number-damping stochastic projected Gross-Pitaevskii equation (4.27) or the full stochastic projected Gross-Pitaevskii equation (3.93). Our goal is to determine if these two closely related theories give different results, and if so explain the difference.

4.5.1 Dimensionless Units

We work in harmonic oscillator units set by the transverse trapping frequency of our system, the value of which is chosen as $\omega_{\perp}/2\pi = 200\text{Hz}$. The dimensionless units are

$$x_0 = a_{\perp} = \sqrt{\frac{\hbar}{m\omega_{\perp}}}, \quad t_0 = \frac{ma_{\perp}^2}{\hbar} = \frac{1}{\omega_{\perp}}, \quad E_0 = \frac{\hbar^2}{ma_{\perp}^2} = \hbar\omega_{\perp}.$$

Conveniently this unit choice means that the dimensionless system size L is also the anisotropy. A common choice of natural units used in simulating Bose gases is based on the healing length and speed of sound in the condensate. However the very nature of the dynamics being simulated mean that these quantities are time-dependent rendering them inappropriate for use here.

4.5.2 Simulation Parameters

We use parameters consistent with the atomic species rubidium-87, commonly used in experiments involving Bose-Einstein condensation. These parameters include the mass $m = 87u$, where u is the atomic mass unit, and the s-wave scattering length $a_s = 100a_0$ where a_0 is the Bohr radius. Both these parameters along with the transverse trapping frequency, are used in determining the interaction parameter $g_1 = 2\hbar\omega_{\perp}a_s$. The chosen parameters result in the dimensionless value of the interaction parameter being $g_1 = 0.0139\hbar\omega_{\perp}a_{\perp}$.

We consider a system of length $L = 200a_{\perp}$ simulated on a grid consisting of $M = 1024$ points with periodic boundary conditions. The chemical potential is quenched from $\mu = -\hbar\omega_{\perp}$ to $\mu = \hbar\omega_{\perp}$, that is, $\mu_0 = E_0$ in (4.24). The time over which the quench takes place is thus $t \in [-\tau_Q, \tau_Q]$. The temperature is held constant throughout all simulations at $T = 0.5T_c$ where T_c is the transition temperature for the ideal Bose gas in a box potential of length L , embedded in a 3D thermal cloud where the two tightly confined directions are harmonically trapped. It can be shown [89] that this critical temperature is given by

$$T_c = \frac{\hbar\bar{\omega}}{k_B} \left(\frac{N}{\zeta(5/2)} \right)^{2/5} \quad (4.51)$$

with $\bar{\omega}$ the modified geometric mean frequency

$$\bar{\omega}^5 = \frac{2\pi\hbar}{mL^2}\omega_{\perp}^4, \quad (4.52)$$

and N the number of particles. To calculate the critical temperature T_c we have used the Thomas-Fermi value of N

$$N = \frac{\mu}{g_1}L \quad (4.53)$$

corresponding to the post-quench parameters, which gives a particle number of $N \approx 14400$. For the number-damping sub theory these parameters give an average **C**-field population of $N_{\mathbf{C}} \approx 14300$ and condensate number $N_0 \approx 12600$ for the final chemical potential $\mu = \hbar\omega_{\perp}$, while the inclusion of energy-damping drops these values to $N_{\mathbf{C}} \approx 13100$ and $N_0 \approx 10200$. The quench times τ_Q were chosen such that the fast quench limit could be observed, but not so slow that a second regime is entered where the winding obeys a different power law [90].

For obtaining the initial state of the system, a number-damping rate of $\gamma = 1$ is used. This is equivalent to evolving in imaginary time, and will rapidly damp any initial wave function ansatz to the correct equilibrium state at temperature T . A more realistic value for the damping rates in experiments involving dynamics is $\mathcal{O}(10^{-4})$ (see e.g. [4]), however we can use a larger value provided the resultant time scale remains much larger than any other time scales present in problem. We choose a value for the dimensionless number-damping rate of $\gamma = 10^{-2}$, implemented once the correct initial equilibrium state is reached. For the number-damping SPGPE, the energy-damping is not included, so an energy-damping rate of $\mathcal{M} = 0$ is used for the entirety of the simulation. For the full SPGPE, we include energy-damping and choose the energy-damping rate $\mathcal{M} = 10^{-2}$ for the entirety of the simulation. Thus, after the initial equilibrium is reached, the number-damping and energy-damping rates have the same magnitude.

Each trajectory is composed of three stages. We now give a summary of the purpose of each stage, and the parameter changes that are implemented in achieving it.

Initial Equilibration

The first stage is allowing the system to come to equilibrium for the initial chemical potential $\mu = -\hbar\omega_{\perp}$. We start with the initial **C**-field wave function $\psi_{\mathbf{C}}(x) = 0$ and rely on the number-damping noise and dissipation to evolve the system to thermal equilibrium. To this end we hold the chemical potential at $\mu = -\hbar\omega_{\perp}$ and evolve with a high number-damping rate of $\gamma = 1$ for 1000 units of the relaxation time, defined by (4.42). We have found that extending this time has no effect on the **C**-field properties. Thus, after this period of evolution, the **C**-field has populated and thermalised to the equilibrium state defined by the reservoir temperature T and chemical potential μ . The time elapsed during this stage is $t = 1000\omega_{\perp}^{-1}$.

Chemical Potential Ramp

The second stage is performing the quench itself. The number-damping rate is changed abruptly to the more realistic value of $\gamma = 10^{-2}$. The chemical potential ramp, given by (4.24), is then started; the chemical potential increases linearly until the final value of $\mu = \hbar\omega_{\perp}$ is reached. The time elapsed during this stage is $t = 2\tau_Q$, where τ_Q is varied between $10^4\omega_{\perp}^{-1}$ and $10^8\omega_{\perp}^{-1}$.

Final Equilibration

The third stage is allowing the system to come to a new equilibrium. Because the post-quench dynamics may prove to be important, we do not increase the number-damping rate as in the first stage, but instead leave it at the value $\gamma = 10^{-2}$. The system is left to evolve with the final chemical potential $\mu = \hbar\omega_{\perp}$ for 10 units of the relaxation time. We have found that post-quench dynamics have ceased by this point, and increasing the equilibration time has no effect on the $\mathbf{C}$ -field properties. The time elapsed during this stage is $t = 1000\omega_{\perp}^{-1}$.

The data we obtain from these trajectories can be divided into two categories. One category is the data which requires the construction of the one-body density matrix to obtain; this includes the correlation length, condensate number, and condensate wave function. Thus to obtain this data over the course of an ensemble of trajectories we must construct the one-body density matrix at each time step, a task that increases the required computation time for each trajectory. However constructing the one-body density matrix requires taking an ensemble average over trajectories, and hence there must be sufficient trajectories to obtain the one-body density matrix at all. We have performed 1000 trajectories for each parameter set to obtain the one-body density matrix over time. We found that this number was sufficient to obtain a one-body density matrix that is relatively free of sampling error.

The second category is the data which does not require the one-body density matrix; of particular interest to us is the winding of the system. Since there is no computational time spent on constructing the one-body density matrix, a much larger ensemble of trajectories may be performed with the same total computational time. This is fortunate, as the winding distribution converges significantly slower than the ensemble averaging of the one-body density matrix, thus requiring a much larger number of trajectories¹. We have performed 10000 trajectories for each parameter set to obtain the winding of the system over time. We found that this number was sufficient to obtain statistics of the winding distribution with relatively small error.

4.5.3 Numerical Implementation

The number-damping SPGPE is solved numerically using an adaptive Runge-Kutta method in the interaction picture [91, 92]. The numerical implementation of the number-damping SPGPE has been previously outlined [12, 93]. The Runge-Kutta method may be applied to the number-damping SPGPE as it relies on the noise being additive. The presence of multiplicative noise in the full SPGPE means we must resort to a different algorithm for finding numerical solutions. The full SPGPE (3.93) is solved numerically using a weak semi-

¹In particular we are interested in the winding standard deviation, the error of which scales like $N^{-1/2}$, where N is the number of trajectories. The ensemble averaging to obtain the density matrix is essentially taking the mean over a number of trajectories, the error of which scales like N^{-1} .

implicit Euler method, the details of which can be found in [7, 65]. The time step should be smaller than any other time scale in the problem, and as such we choose the value $dt = 0.02\omega_{\perp}^{-1}$. The weak semi-implicit Euler algorithm converges to a solution significantly slower than the Runge-Kutta method, and as such numerical trajectories of the full SPGPE take significantly more computation time than the equivalent trajectories of the number-damping SPGPE. The precise details of numerical implementation of the SPGPE is not a key topic of this thesis, and we refer the reader to [12, 91–93] for the number-damping SPGPE method, and [7, 65] for the full SPGPE method.

Our simulations required a large amount of computing resources. Large arrays of data, up to 10000×1024 complex elements in size, were required to represent the ensemble of trajectories being simulated. Our research group at the University of Otago has recently obtained two NVidia Tesla K40 GPU Accelerators, which are an excellent resource for parallel computing. We used one of these GPUs to perform the vast majority of our simulations, with some being performed on the University of Otago Vulcan cluster. The time required for simulating a particular ensemble of trajectories was dependent on the quench rate, with the slowest quench rate taking ~ 120 hours to obtain 10000 trajectories. Large amounts of storage space was also required to hold our data, the total size of which was $\sim 1.5\text{TB}$.

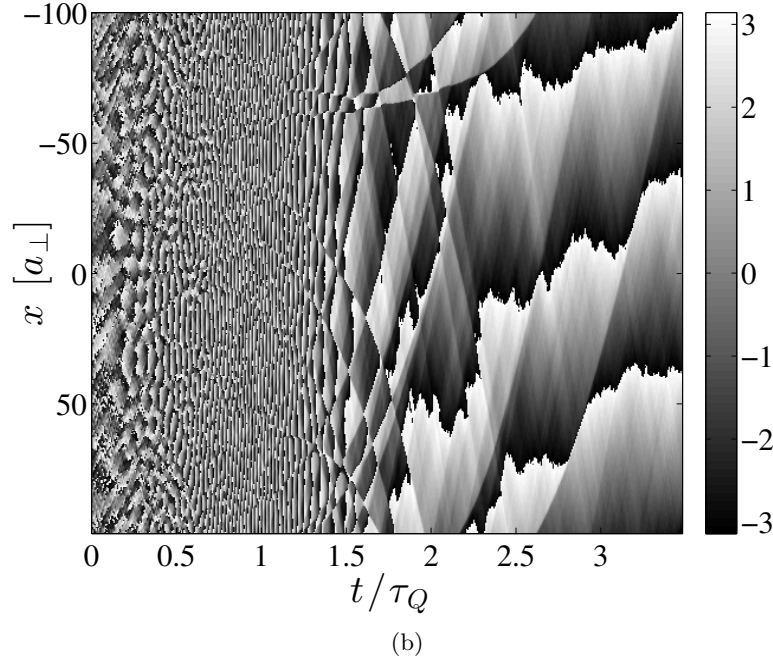
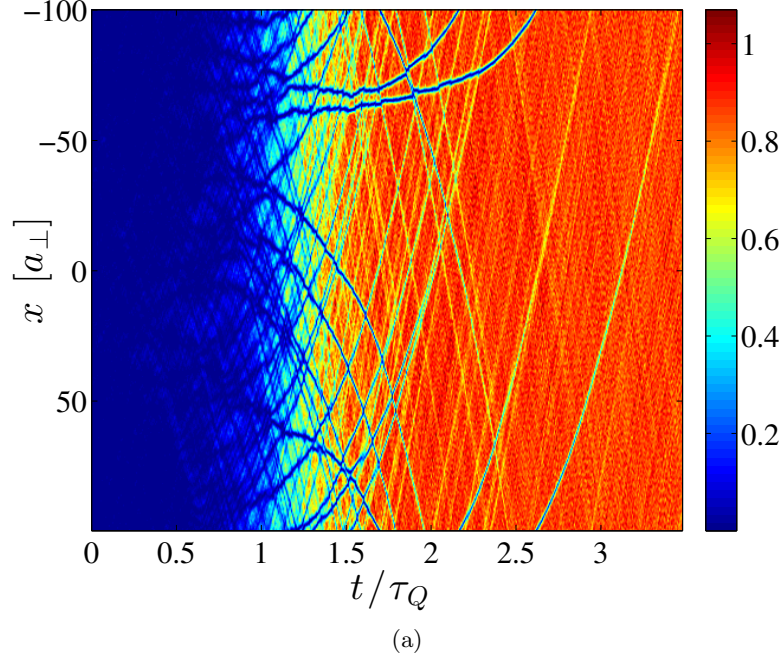


Figure 4.2: Number density (a) and phase (b) of the $\mathbf{C}$ -field during a typical quench. Note that during initial density growth there are numerous solitons, evident as low-density notches with an associated phase jump, but by $\sim 3\tau_Q$ after the transition they have almost all decayed. The value of $\sim 3\tau_Q$ is not universal; faster and slower quenches have differing times at which all solitons have decayed. The phase plot reveals that a final winding of 3 has been acquired, shown by the 3 jumps of 2π .

4.6 Quench Simulations

In this section we present the various results we have obtained from our quench procedure. For each piece of data we will explain how it was extracted, how the results of the two theories differ, and how they compare to the mean-field predictions. An example of a typical quench is shown in Figure 4.2, where one can see the formation and subsequent instability of the dark solitons resulting from the merging of independently phased domains. Some characteristics of solitons can be inferred such as the inverse relationship between speed and depth, and collisions. From this point on, we will use a different terminology to refer to the two theories we are implementing. Theory γ (gamma) will refer to the number-damping SPGPE (4.27), while theory ε (epsilon) will refer to the full SPGPE (3.93).

4.6.1 Condensate Number Growth

If the system were allowed to evolve adiabatically throughout the entire quench, the condensate number would simply grow linearly with the chemical potential after the critical point had been passed. However the adiabatic-impulse approximation insists that when the system is in the impulse regime, the dynamics are frozen and thus the condensate number must be unable to grow. Once the system is released from the impulse regime, non-equilibrium dynamics will take place as the condensate number rapidly grows. Therefore we expect to see that, at the boundary between the impulse and adiabatic regimes ($t = \hat{t}$), there is a kink in the condensate number. If we look at the condensate number as a function of time $N_0(t)$ for a variety of quench rates, then rescaling the time axis by $\hat{t}$ should result in all of the kinks lying on top of one another, providing a confirmation of universal KZM scaling.

The condensate number is found using the Penrose-Onsager criterion at each time step [94]. The one-body density matrix is found using

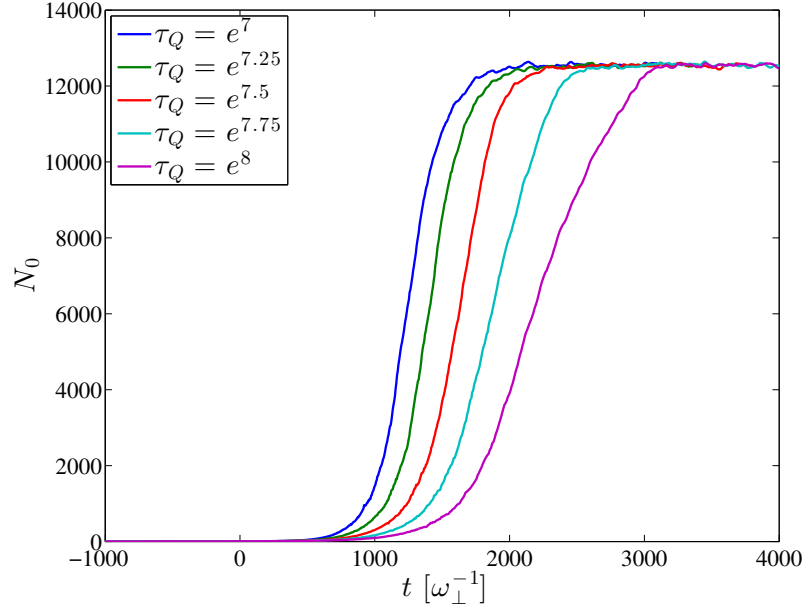
$$\rho(x, x') = \langle \psi_{\mathbf{C}}^*(x) \psi_{\mathbf{C}}(x') \rangle \quad (4.54)$$

where the angled brackets denote ensemble averaging over a number of trajectories. Solving the eigenproblem

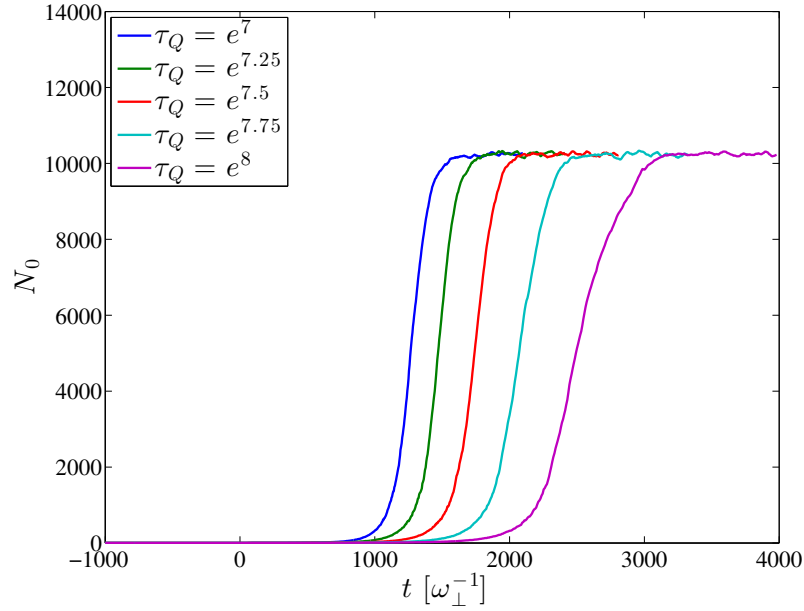
$$\int dx' \rho(x, x') \phi_k(x') = n_k \phi_k(x). \quad (4.55)$$

then gives the eigenvalues n_k and eigenfunctions $\phi_k(x)$, where $\phi_k(x)$ are the system orbitals and n_k their occupation. The largest eigenvalue

$$N_0 \equiv \sup_k n_k. \quad (4.56)$$



(a)



(b)

Figure 4.3: The condensate number over time for several quench times using theory γ (a) and theory ε (b). The condensate number was extracted using the Penrose-Onsager criterion (4.56).

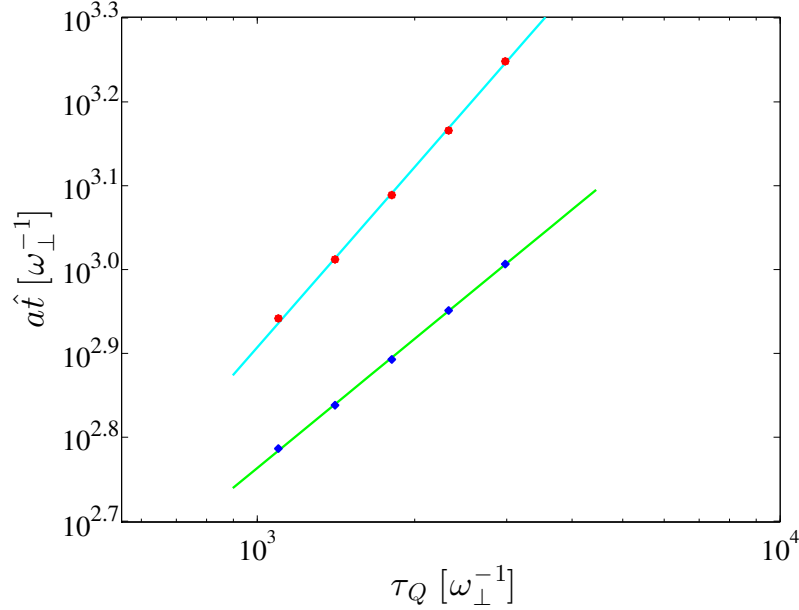


Figure 4.4: The results of our self-similarity algorithm with respect to the condensate number for theory γ and theory ε . The numerical data for theory γ (theory ε) is represented by blue (red) points, while the green (cyan) line is a least squares fit of a power law to the numerical data. The power law exponents are $\alpha = 0.5119 \pm 0.0178$ and $\alpha = 0.7145 \pm 0.0358$ for theory γ and theory ε respectively.

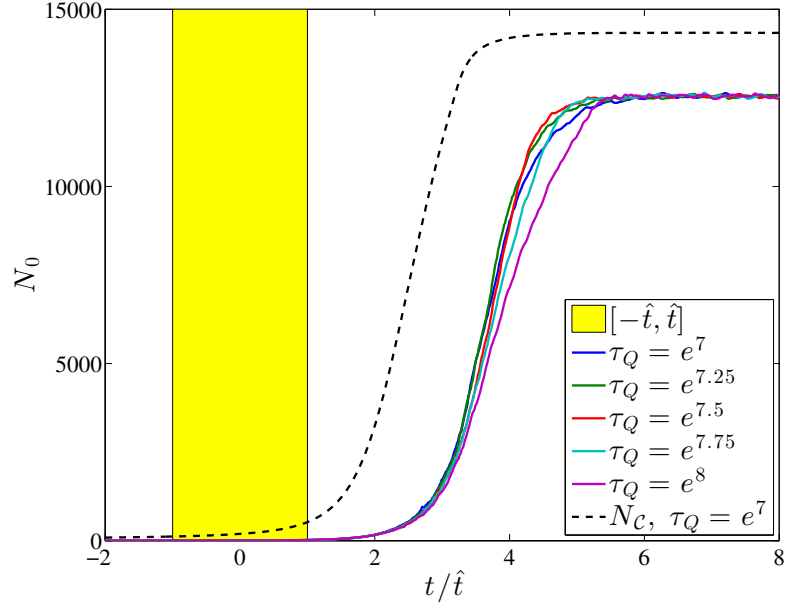
gives the condensate number N_0 and associated wave function $\phi_0(x)$.

The mean condensate number for several quenches is shown in Figure 4.3. The curves appear to be of the same functional form, but with the time axis scaled. This property is known as *self-similarity*, where rescaling the time axis by a particular factor will cause the curves to collapse onto one universal curve. The rescaling factor that causes the curves to collapse onto one another is the freeze-out time, as discussed above. We use an algorithm to find the freeze-out time from these curves based on their self-similarity; we refer to this as our *self-similarity algorithm*, and we now describe how it is implemented. A reference condensate number is chosen relatively close to where the condensate number initially grows. The time at which this reference is reached should be linearly proportional to the freeze-out time, and thus obey a power law also

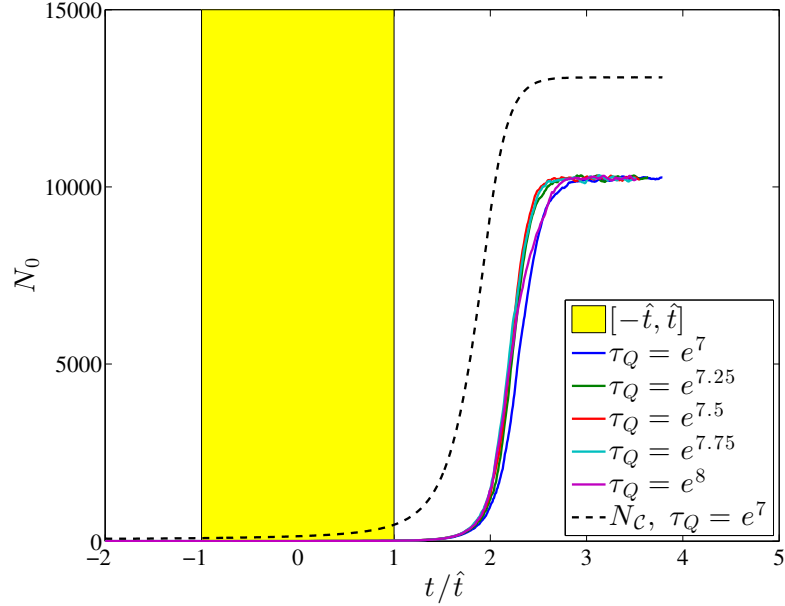
$$a\hat{t} = a (\tau_0 \tau_Q^{z\nu})^{\frac{1}{1+z\nu}}, \quad (4.57)$$

where a is a constant of order unity. We then use a power-law fit to obtain the power-law exponent α (4.8) of the quench time τ_Q and thus the value of $z\nu$. This allows us to determine the actual freeze-out time using (4.7) with the constants ξ_0 (4.43) and τ_0 (4.44).

We use a reference condensate number of $N_0 = 100$, occurring rapidly after initial condensate growth. Figure 4.4 shows the time at which the reference condensate number is reached



(a)



(b)

Figure 4.5: The condensate number over time for several quench times using theory γ (a) and theory ε (b). The time axis has been scaled by the freeze-out time as predicted by our self-similarity algorithm for each theory. The yellow shaded region indicates the impulse regime where KZM approximates the system dynamics as frozen. For comparison, the total **C**-field population is also shown for one of the quenches (black dashed line).

against the quench time for several different quenches, using both theory γ and theory ε . We can see that both theories give results that obey a power law, with the power law exponent differing between the theories. A least-squares-fit to the results of simulations using theory γ gives a power law exponent of $\alpha = 0.5119 \pm 0.0178$, which compares favourably with the mean field prediction $\alpha = 0.5$. A least-squares-fit to the results of simulations using theory ε gives a power law exponent of $\alpha = 0.7145 \pm 0.0358$, a value which is distinctly outside the mean field prediction. The product $z\nu$ determined by these values of α is $z\nu = 1.048 \pm 0.075$ for theory γ (compared to $z\nu = 1$ for mean field) and $z\nu = 2.503 \pm 0.439$ for theory ε .

The mean condensate numbers over the course of several quenches in the power law regime are shown in Figure 4.5 with the time axis now rescaled by the freeze-out time using the values of $z\nu$ predicted by the self-similarity algorithm as stated above. The impulse regime $t \in [-\hat{t}, \hat{t}]$ is highlighted to emphasise that condensate growth does not begin until the system has entered the adiabatic regime. We see that rescaling the time axis by $\hat{t}$ does result in the kinks lying on top of one another, for both theory γ (Figure 4.5a) and theory ε (Figure 4.5b). The condensate does not rapidly populate immediately upon release from the impulse regime ($t = \hat{t}$), but instead initially exhibits slow growth until $t \approx 3\hat{t}$ for theory γ and $t \approx 2\hat{t}$ for theory ε . At this point the condensate rapidly grows until equilibrium is reached; this behaviour is consistent with quantum kinetic theory [60]. We have also included for comparison the growth of the **C**-field particle number $N_{\mathbf{C}}(t)$ for one value of the quench time for comparison. As one would expect the **C**-field particle number is always greater than the condensate number. Interestingly the **C**-field particle number does exhibit some growth in the impulse regime, suggesting that the system dynamics may not be totally frozen.

Apart from the differing power law exponents, there are some other differences between the condensate number growth dynamics for the two theories. The equilibrium values of the condensate number and **C**-field number are lower for theory ε than for theory γ . This is possibly due to the presence of an extra noise source creating a higher effective temperature of the system. In addition, the slope of the condensate number curve during the period of rapid growth is greater for theory ε than for theory γ , indicating a faster route to equilibrium.

4.6.2 Correlations

For all times prior to the transition at $\mu = 0$, we are free to use equation (4.50) as a fit to obtain the freeze-out correlation length $\hat{\xi}$, then use this value and equation (4.49) as a fit to obtain the correlation length as a function of time. Using equations (4.50) and (4.49) relies on the interaction term $g_1|\psi_{\mathbf{C}}|^2$ being negligible, thus they fail once the **C**-field occupation is significant. In Figure 4.6 we compare the analytic form of the freeze-out correlation function (4.50) with the numerically extracted correlation function from simulations of theory γ at $t = -\hat{t}$ and $t = \hat{t}$, with $\hat{t}$ given by (4.7) and mean-field critical exponents. It was seen in the previous section that the numerically obtained freeze-out time fell within error of that given by

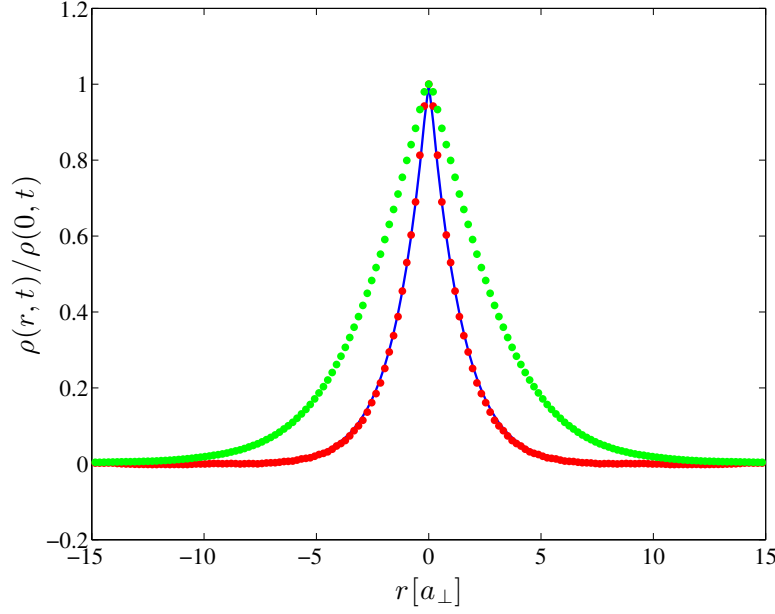


Figure 4.6: The correlation function at $t = -\hat{t}$ (red dots) and $t = \hat{t}$ (green dots) for a quench simulated using theory γ . The analytic form (blue) is given by (4.50) normalised to one by dividing by its maximum value $\rho(0, \hat{t})$. The numerical result is found by calculating the density matrix with 1000 trajectories and averaging over one of the spatial dimensions, before normalising by dividing by its maximum value.

mean-field critical exponents. The correlation function is found numerically by constructing the density matrix at each point in time for 1000 trajectories of the quench, then averaging over one of the spatial dimensions, thus making use of the translational invariance of the density matrix.

We see that equation (4.50) describes the correlation function very well at $t = -\hat{t}$, but fails to show any agreement for $t = \hat{t}$. This is not so surprising, as the assumptions made in deriving (4.50) are no longer valid at $t = \hat{t}$ due to the growing $\mathbf{C}$ -field density. Inspecting equation (4.49) we see that it must fail once the correlation length is appreciably greater than $\hat{\xi}$ as the second argument of the function $f(x, y)$ goes to zero for $\xi(t) \gg \hat{\xi}$, ridding it of any time dependence. That is, equation (4.49) can only predict a growing correlation length up to values on the order of $\hat{\xi}$, after which it will admit any arbitrarily large value of $\xi(t)$. In fact, Figure (4.6) shows that the correlation length has not grown by too much between $-\hat{t}$ and $\hat{t}$, yet (4.49) is already disagreeing significantly. This suggests that if we wish to investigate the correlation length over the course of a quench, we will need a method other than fitting to (4.49).

A crude estimate of the correlation length at any point in time is to assume the correlation

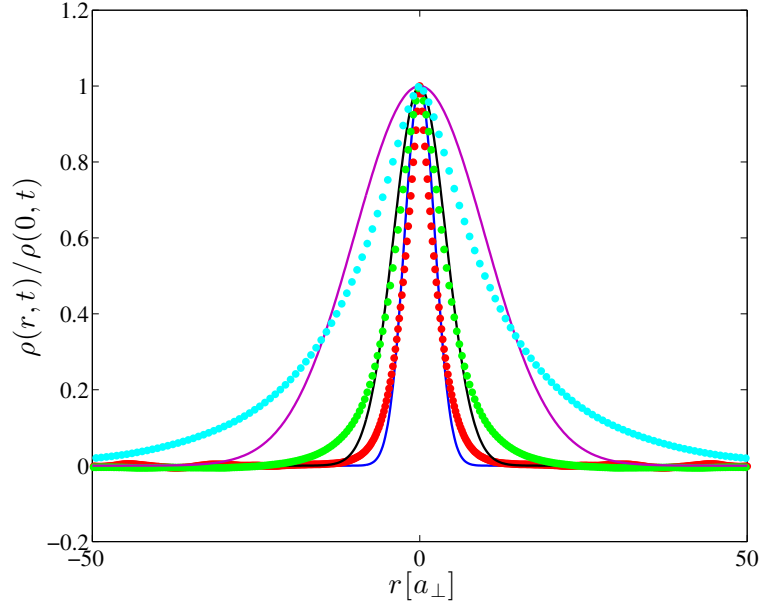


Figure 4.7: The correlation function at $t = \hat{t}$ (red dots), $t = 2\hat{t}$ (green dots), and $t = 3\hat{t}$ (cyan dots) for a quench simulated using theory γ . The solid lines are best fits of (4.58) to the correlation function at $t = \hat{t}$ (blue), $t = 2\hat{t}$ (black), and $t = 3\hat{t}$ (magenta). The numerical result is found by calculating the density matrix with 1000 trajectories and averaging over one of the spatial dimensions, before normalising by dividing by its maximum value.

function can be approximated by

$$\langle \psi_{\mathbf{C}}^*(x, t) \psi_{\mathbf{C}}(x', t) \rangle \approx A e^{-\frac{(x-x')^2}{\xi(t)^2}} \quad (4.58)$$

where A is an arbitrary constant². To ensure that this approximation is valid, we compare the correlation length at $t = -\hat{t}$ as given by fitting to (4.50) to that given by fitting to (4.58). The approximation will be suitable provided it gives the same scaling with τ_Q ; getting the magnitude exactly right is less important, provided they differ from each other by a constant factor. In other words, the approximation should be valid provided

$$\hat{\xi}_1 \approx \lambda \hat{\xi}_2 \quad (4.59)$$

where $\hat{\xi}_1$ is the numerical freeze-out correlation length resulting from fitting to (4.50), $\hat{\xi}_2$ is the numerical freeze-out correlation length resulting from fitting to (4.58), and λ is some constant factor.

Figure 4.9a is a log-log graph comparing the numerically obtained values $\hat{\xi}_1$ and $\hat{\xi}_2$. Dif-

²We also investigated using a decaying exponential fit, as opposed to the Gaussian, however the same critical behaviour of the correlation length was observed. In addition, the Gaussian fit gave a correlation length at $t = -\hat{t}$ closer to the analytic result (4.47) than the decaying exponential fit.

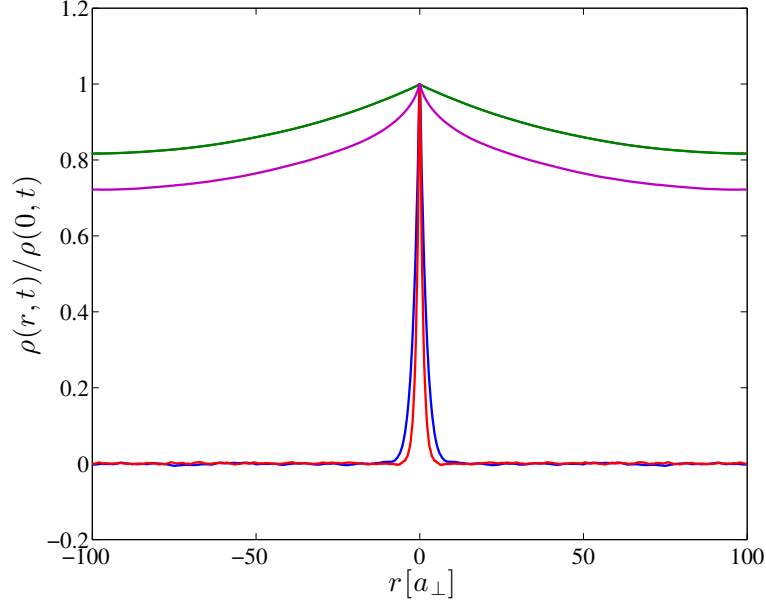


Figure 4.8: The correlation function at the phase transition (blue) and after reaching equilibrium post-quench (green) for a quench simulated using theory γ , and the correlation function at the phase transition (red) and after reaching equilibrium post-quench (magenta) for a quench simulated using theory ε . The correlation function is found by calculating the density matrix with 1000 trajectories and averaging over one of the spatial dimensions, before normalising by dividing by its maximum value.

fering by a constant factor λ will manifest in this plot as a constant vertical shift. The values $\hat{\xi}_1$ and $\hat{\xi}_2$ appear upon inspection to differ by a constant factor as hoped. We can verify this by looking at the percentage difference between $\hat{\xi}_1$ and $\lambda\hat{\xi}_2$, where we estimate λ as the mean value of $\hat{\xi}_1/\hat{\xi}_2$. This is shown in Figure 4.9b, where we see that the percentage difference is never greater than 1.5% for the quench times we are investigating. We also show in Figure 4.7 the correlation function at various times after the transition, along with the corresponding least-squares-fit to (4.58). We can see the fit is somewhat appropriate for the correlation function at $t = \hat{t}$ and $t = 2\hat{t}$ when the function is still large, but shows disagreement when the function approaches zero. In addition, the fit at $t = 3\hat{t}$ shows significant disagreement with the data. However the fit will still give us a measure of the correlation function width. We can thus conclude that using equation (4.58) to estimate the value of the correlation length is an appropriate procedure. We will use equation (4.50) only when we are looking at the correlation length specifically at the negative freeze-out time, $t = -\hat{t}$.

In Figure 4.8 we show the correlation function at the phase transition and after reaching equilibrium post-quench for quenches simulated using both theory γ and theory ε . As we would expect, the correlation length exhibits significant growth after the phase transition. The correlation length from theory γ is greater than that from theory ε , presumably due to

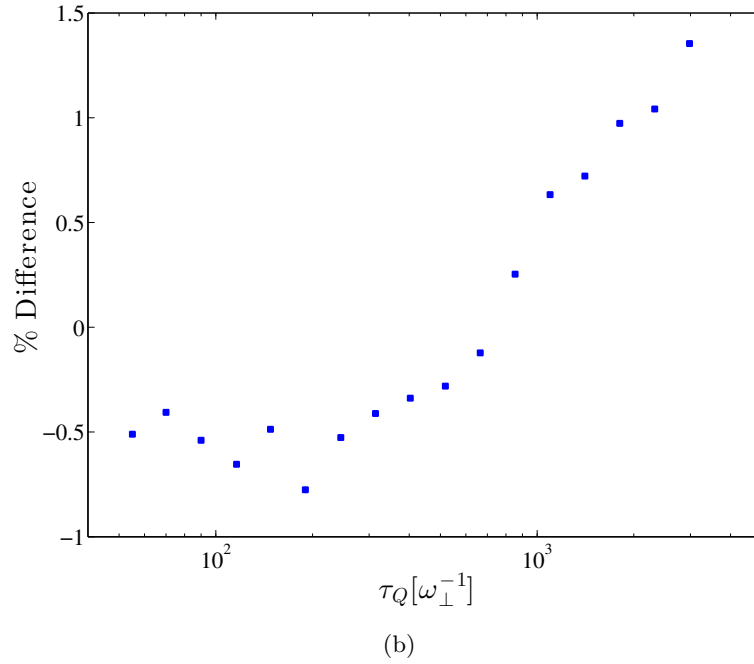
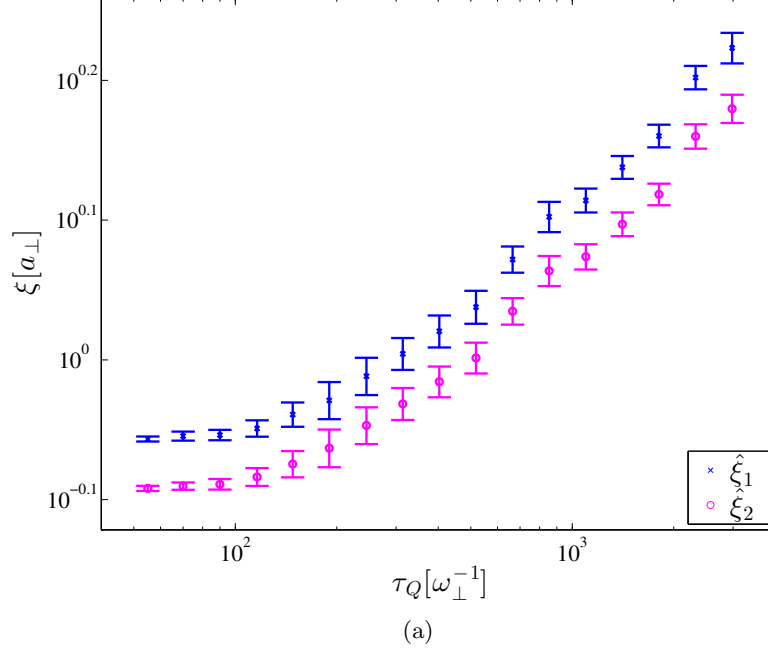


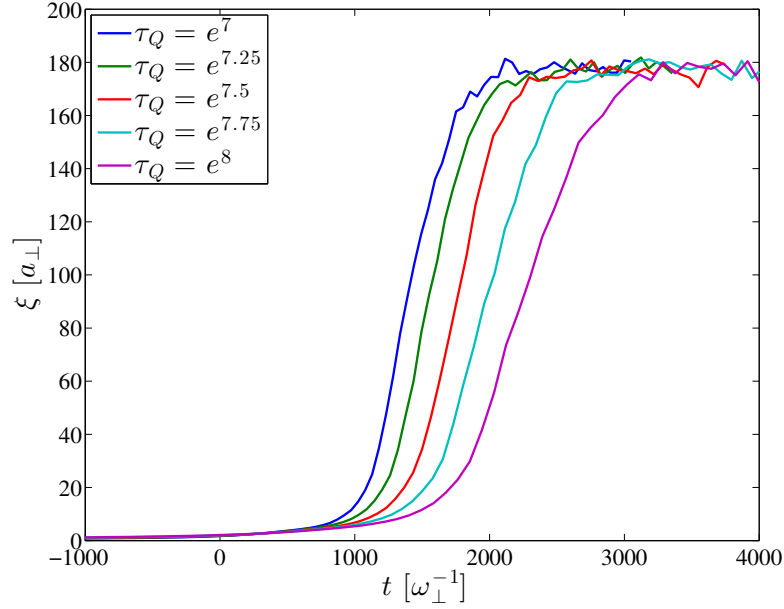
Figure 4.9: (a) The correlation length at $t = -\hat{t}$ as given by fitting to equation (4.50) ($\hat{\xi}_1$, blue crosses) or equation (4.58) ($\hat{\xi}_2$, magenta circles). Here the axes are log-log, so a constant factor difference becomes a vertical shift. (b) The percentage difference between $\hat{\xi}_1$ and $\lambda\hat{\xi}_2$ relative to $\hat{\xi}_1$, where λ is the mean of $\hat{\xi}_1/\hat{\xi}_2$. The data shown here was obtained using theory γ , with the value of $\hat{t}$ given by mean field critical exponents.

the extra noise source. In the new equilibrium states, we see that the correlation function has decayed by much less than half the initial value at its full extent. This implies that the final correlation length may be expected to be at least on the order of the system size.

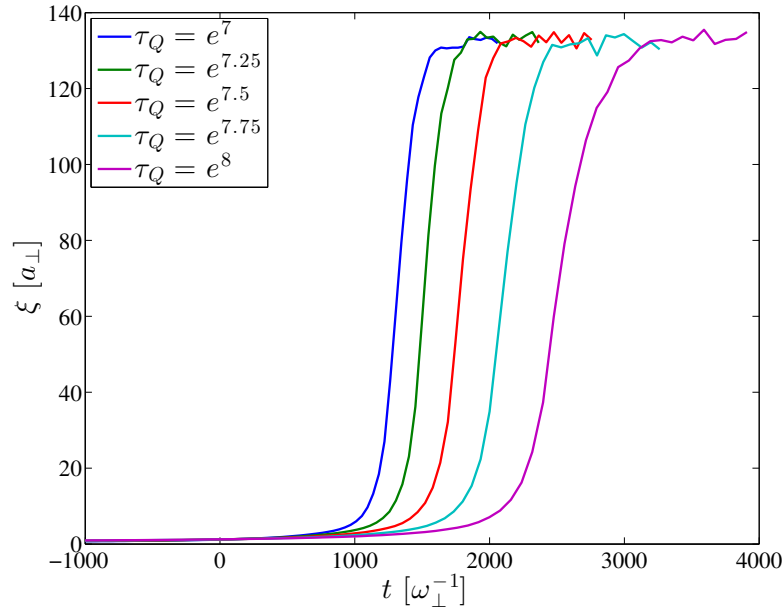
The correlation length over the course of several quenches in the power law regime are shown in Figure 4.10. The curves show promising signs of self-similarity where the correlation length begins to increase, that is, they appear that they may be of the same functional form but with the time axis scaled. The rescaling factor that causes the curves to collapse onto one another is the freeze-out time, as discussed with respect to the condensate number in the preceding subsection. We again use a self-similarity algorithm, choosing a reference correlation length prior to reaching final equilibrium and finding the time at which this value is reached for each quench. This time should obey a power law with respect to the quench time, thus we use a least squares fit to obtain the exponent $\alpha = z\nu/(1 + z\nu)$ and hence the value of $z\nu$ allowing us to determine the actual freeze-out time.

A relatively large reference correlation length is required here as the relative error becomes large for the values of the correlation length close to zero. We use a reference correlation length of $\xi = 60a_{\perp}$. Figure 4.11 shows the time at which the reference correlation length is reached against the quench time for several different quenches, using both theory γ and the theory ε . We can see that both theories give results that obey a power law, with the power law exponent differing between the theories. A least squares fit to results of theory γ gives a power law exponent of $\alpha = 0.5118 \pm 0.0357$, which compares favourably with the mean field prediction $\alpha = 0.5$. A least squares fit to the results of theory ε gives a power law exponent of $\alpha = 0.6729 \pm 0.0364$, a value which is distinctly outside the mean field prediction. The product $z\nu$ as determined by these is $z\nu = 1.048 \pm 0.150$ for theory γ (compared to $z\nu = 1$ for mean field) and $z\nu = 2.057 \pm 0.340$ for the theory ε . Both these values are within error of the values obtained using the self-similarity algorithm with respect to the condensate number growth, however we do note the larger error in the results of this procedure.

The correlation length over the course of several quenches in the power law regime are shown in Figure 4.12 with the time axis now rescaled by the freeze-out time using the values of $z\nu$ predicted by the self-similarity algorithm as stated above. The impulse regime $t \in [-\hat{t}, \hat{t}]$ is highlighted to emphasise that the correlation length does not exhibit an appreciable amount of growth until the system has entered the adiabatic regime. We see that rescaling the time axis by $\hat{t}$ does result in the correlation length curves lying on top of one another for both theory γ (Figure 4.12a) and theory ε (Figure 4.12b), with the best agreement evident close to the period of initial growth. The growth of correlation length is not immediate upon release from the impulse regime ($t = \hat{t}$), but instead exhibits slow growth until $t \approx 3\hat{t}$ for theory γ and $t \approx 2\hat{t}$ for theory ε . At this point the correlation length rapidly increases until equilibrium is reached. In addition, the growth of the correlation length is more rapid in theory ε . The post quench equilibrium correlation length is lower for theory ε than theory γ due to the extra



(a)



(b)

Figure 4.10: The correlation length over time for several quench times using theory γ (a) and theory ε (b). The correlation length was obtained at all times by fitting (4.58) to the numerically obtained correlation function.

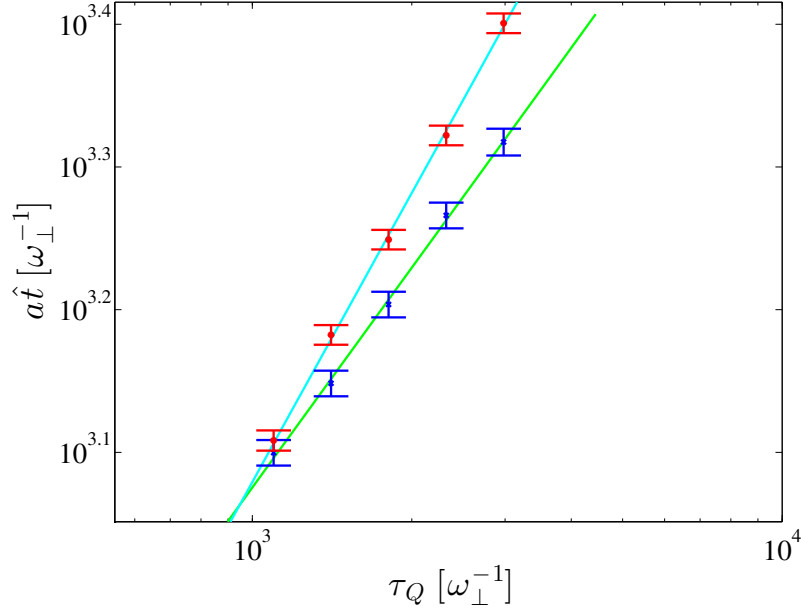
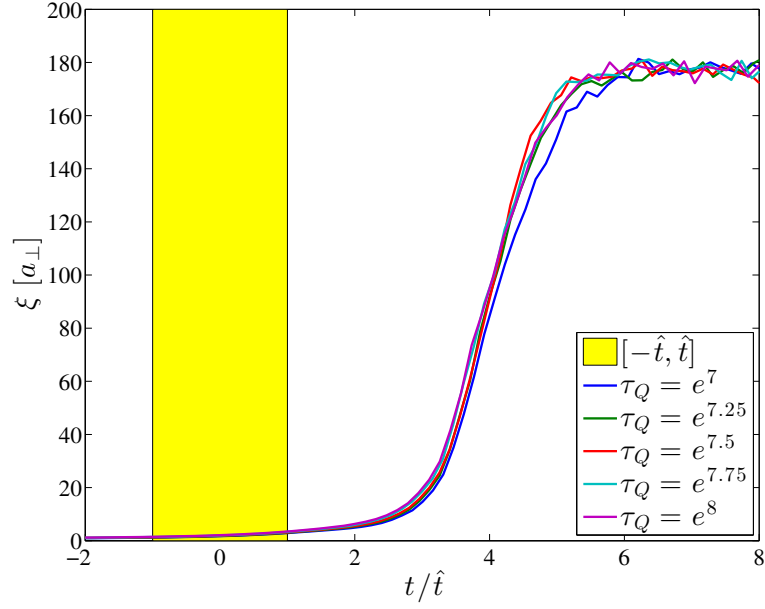


Figure 4.11: The results of our self-similarity algorithm with respect to the correlation length for theory γ and the theory ε . The numerical data for theory γ (ε) is represented by blue (red) points, while the green (cyan) line is a least squares fit of a power law to the numerical data. The power law exponents are $\alpha = 0.5118 \pm 0.0357$ and $\alpha = 0.6729 \pm 0.0364$ for theory γ and theory ε respectively.

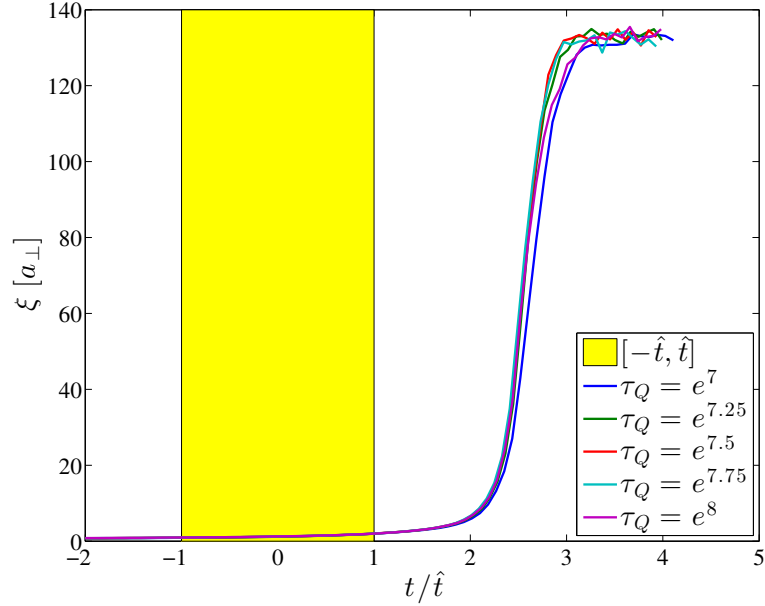
noise source.

We can see from Figure 4.12 that the correlation length does exhibit slow growth within the impulse regime, a clear violation of the adiabatic-impulse approximation. To investigate this we extract the correlation length at the boundaries of the impulse regime and examine how this growth affects the power law scaling. Because the boundaries of the impulse region are not precisely known for theory ε , we do not investigate $\hat{\xi}$ for theory ε as we do not know exactly when $\hat{\xi}$ should occur, limiting this to the results of theory γ only.

In Figure 4.13 we show the numerically extracted correlation lengths for theory γ at both the negative freeze-out time $t = -\hat{t}$ and the positive freeze-out time $t = \hat{t}$, with these values determined by the results of the self-similarity algorithm with respect to the correlation length. We see that the correlation length at $-\hat{t}$ compares well with the mean field prediction far from the fast quench limit. The correlation length at $\hat{t}$ is larger than that at $-\hat{t}$, as can be seen in both Figure 4.12a and Figure 4.6. However the power law with respect to the quench time appears to be essentially unchanged. This may in part explain why predictions of the density of defects (4.11) tend to be an overestimate, requiring that $\hat{\xi}$ be replaced by $f\hat{\xi}$ with $f \sim \mathcal{O}(1 - 10)$ a model-dependent constant [49, 79, 83, 84]. Here the correlation length at $\hat{t}$ is greater than that at $-\hat{t}$ by a factor of $f \approx 2.2$.



(a)



(b)

Figure 4.12: The correlation length over time for several quench times using theory γ (a) and theory ε (b). The time axis has been scaled by the freeze-out time as predicted by our self-similarity algorithm. The yellow shaded region indicates the impulse regime where KZM approximates the system dynamics as frozen. The correlation length was obtained at all times by fitting (4.58) to the numerically obtained correlation function.

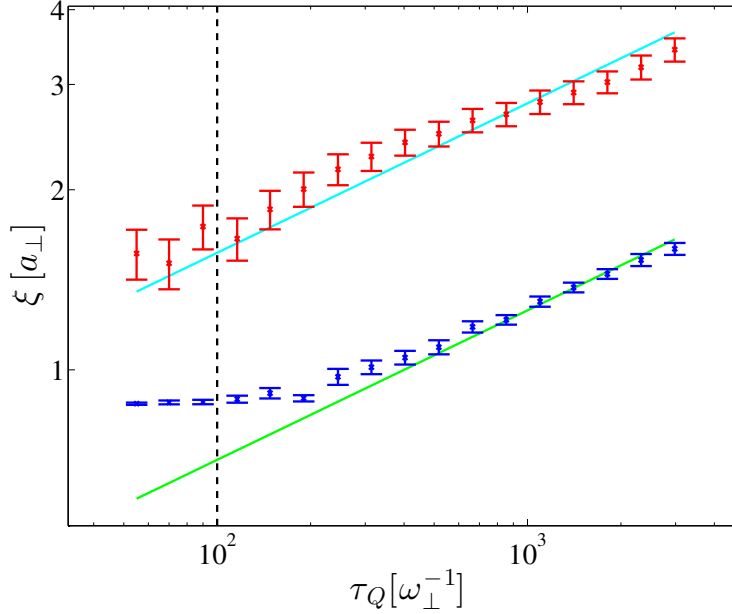


Figure 4.13: Correlation lengths extracted from the density matrix for theory γ . The blue and red crosses are the correlation lengths measured at $-\hat{t}$ and $\hat{t}$ respectively. As discussed in the text, the correlation length at $-\hat{t}$ was obtained by fitting the correlation function to equation (4.50) while at $\hat{t}$ it was obtained by fitting the correlation function to equation (4.58). The green line is the analytic expression (4.10) with mean field critical exponents, while the blue line is a fit with the same power law exponent given here as a guide for the eye. The dashed vertical line represents the fast quench limit (4.13).

4.6.3 Statistics of Final Winding Numbers

For each quench time the standard deviation of the final winding number is calculated from the 10000 trajectories. A regime where a power law appears to be in effect is identified and a least squares fit is used to obtain the power law exponent β (4.23). The fit will also give us the value of f such that replacing $\hat{\xi}$ with $f\hat{\xi}$ results in (4.22) giving the correct magnitude in addition to the power law scaling.

Figure 4.14 shows the standard deviation of the final winding for a range of quench times. We see that far from the fast quench limit ($\tau_m = 10^2$) the winding standard deviation from both the theory γ and theory ε simulations obeys a power law with respect to the quench time. The power law exponent differs between the two; theory γ gives a power law exponent of $\beta = 0.1236 \pm 0.0098$ while theory ε gives a power law exponent of $\beta = 0.0966 \pm 0.0128$. The mean field value $\beta = 0.125$ is within error of the theory γ value, but not within error of the value resulting from theory ε .

The power law fits to the standard deviation can also be used to determine the value of

f for theory γ . The power law predicted by KZM is

$$\sigma(\mathcal{W}) = \sqrt{\frac{L}{6\xi_0}} \tau_0^\beta \tau_Q^\beta = A \tau_Q^\beta \quad (4.60)$$

while including the correcting factor f gives

$$\sigma_f(\mathcal{W}) = \sqrt{\frac{L}{6f\xi_0}} \tau_0^\beta \tau_Q^\beta = A_f \tau_Q^\beta. \quad (4.61)$$

Assuming the factor f is responsible for the discrepancy in magnitudes between our results and (4.60), our results then correspond to (4.61). The numerical value of f can then be determined by

$$f = \left(\frac{A}{A_f} \right)^2 = \frac{L}{6\xi_0} \frac{\tau_Q^{2\beta}}{A_f^2} \quad (4.62)$$

where A_f is obtained from a least-squares-fit of a power law to our data. Applying this procedure leads us to a correcting factor of $f = 10.43 \pm 0.23$. This is of the expected magnitude [49,79,83,84], however it is inconsistent with the value of $f \approx 2.2$ we suggested in the previous subsection; clearly the presence of a correcting factor f cannot be attributed solely to the

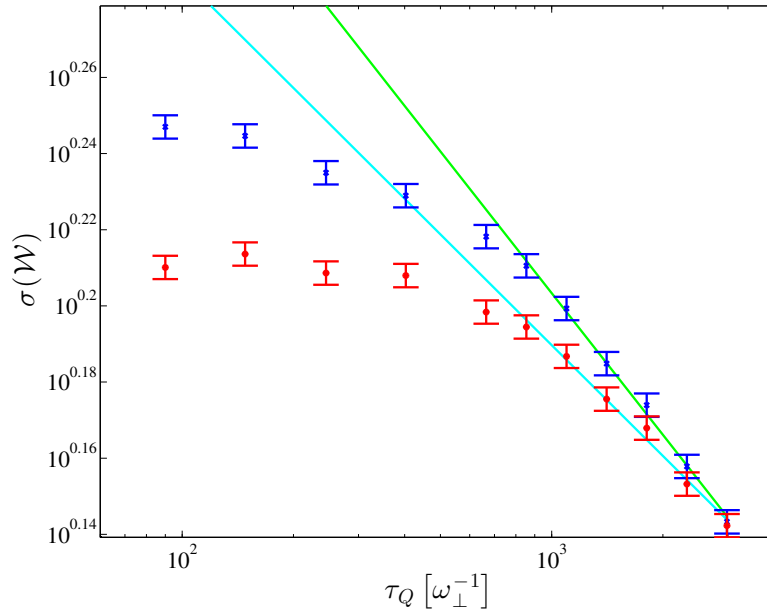


Figure 4.14: Standard deviation of the final winding for various quench times. The blue and red data points are the result of simulations of theory γ and theory ε respectively. The green line is a best fit for the theory γ data in the regime that obeys a power law, giving an exponent of $\beta = 0.1236 \pm 0.0098$. The cyan line is the equivalent for the theory ε data, giving an exponent of $\beta = 0.0966 \pm 0.0128$.

growth of the correlation length in the impulse regime.

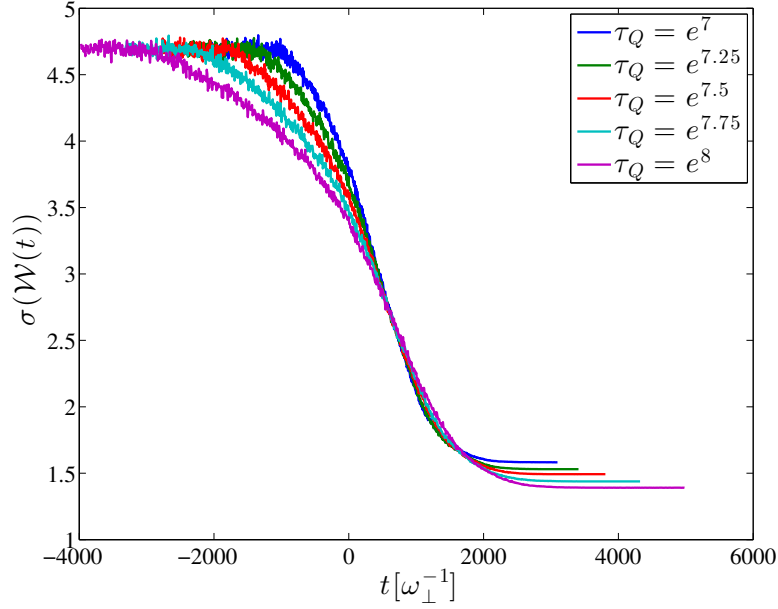
The simulations of theory ε give a winding standard deviation that is always smaller than that obtained via simulations of theory γ for the same quench time. This difference becomes smaller for larger quench times, and the two power laws appear to be converging to a common line at the longest quench considered. Energy damping effects are thought to be most prominent when a system is far from equilibrium, hence we expect that for longer quenches the two theories should converge as the intervals of adiabaticity will be larger compared to the total evolution time.

4.6.4 Dynamical Emergence of Winding

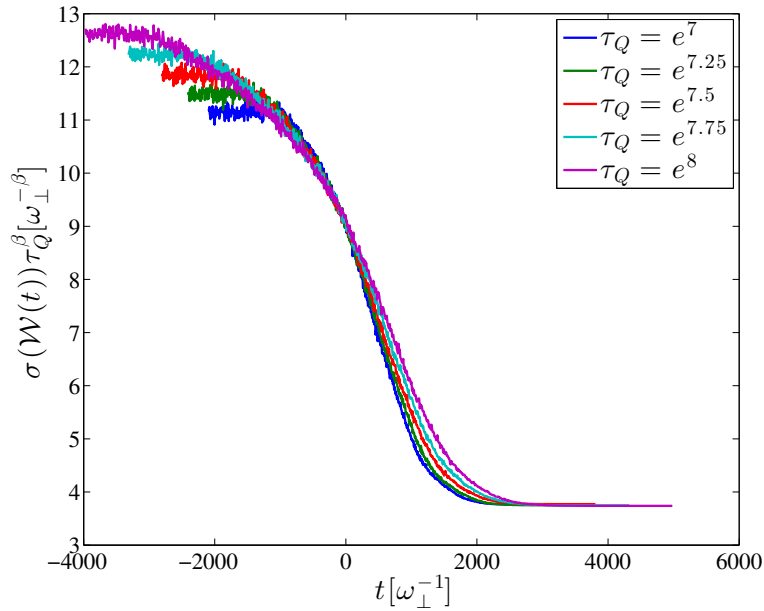
A prediction has already been made for the standard deviation of the winding after post-quench dynamics have ceased, given by equation (4.22). Prior to the cessation of post-quench dynamics, the winding number is still defined as the accumulated phase around the toroid divided by 2π . Thus we can investigate the winding standard deviation over time during the quenches. We investigate the standard deviation of the winding over the course of a quench, for several values of the quench time, for both theory γ and the theory ε .

Figure 4.15a shows the winding standard deviation over time using theory γ for several quench times in the power-law regime. The standard deviation takes the same value initially for every quench time, since each system is prepared in the same initial state. Once the quench is started the standard deviation decreases monotonically until plateauing at a final value. These final values were accurately described by a power law as shown in Figure 4.14. We thus rescale the standard deviation by τ_Q^β with $\beta = 0.1236$, the power law exponent found numerically for the final winding standard deviation. This is shown in Figure 4.15b, where the curves now reach a universal stationary value. Curiously, the curves appear to coincide at $t = 0$, indicating the power law is obeyed there, as well as once the system has reached an equilibrium state. Although we were not looking for or expecting there to be self-similarity along the lines of the condensate number or correlation length, we do see what appears to be promising signs of self-similarity starting at $t = 0$. To investigate this we rescale the time axis by the freeze-out time $\hat{t}$ using the value of $z\nu$ predicted by the self-similarity algorithm with respect to the correlation length ($z\nu = 1.048$). This is shown in Figure 4.16, where we see that, unlike for the correlation length, the rescaling has not resulted in the curves collapsing to a universal value. However, in the vicinity of the transition point ($t = 0$), the curves appear to be well approximated as self-similar. This indicates universal behaviour occurring close to the transition.

Figure 4.17a shows the winding standard deviation over time using theory ε for several quench times in the power law regime. Again the standard deviation begins at a universal value, however we see a jump occur before it decreases to a final value described by the power law shown in Figure 4.14. This jump coincides with the beginning of the quench, as



(a)



(b)

Figure 4.15: The winding number standard deviation over time for several values of the quench time for theory γ . In (a) the standard deviation is left unchanged while in (b) it is scaled by τ_Q^{β} , where β is the value of the standard deviation power law exponent for theory γ , as determined by the results of the final winding statistics.

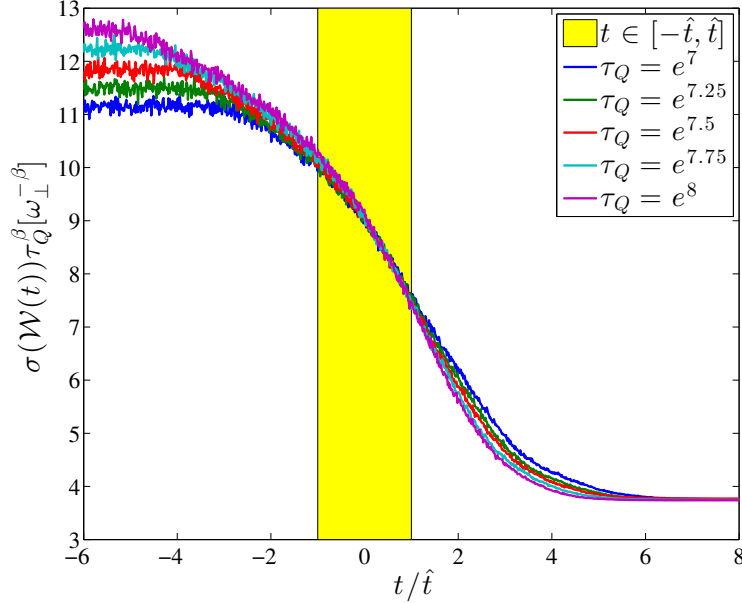
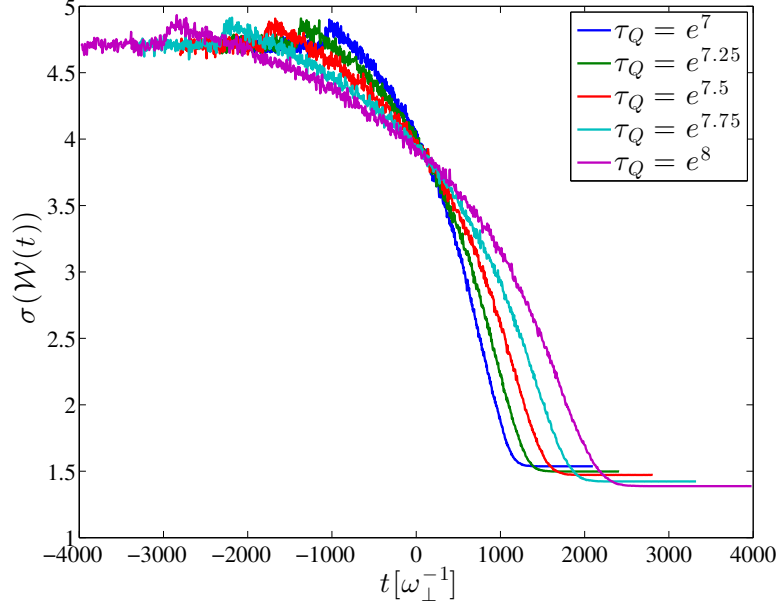
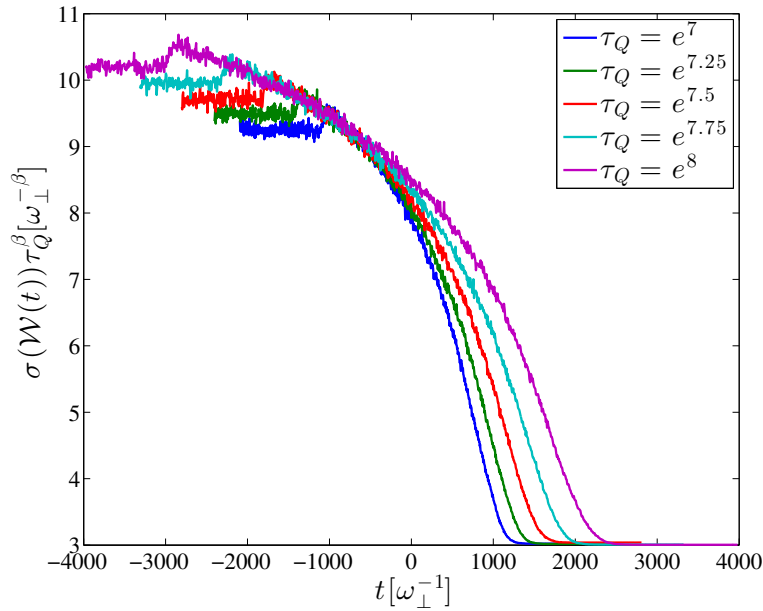


Figure 4.16: The winding number standard deviation over time for several values of the quench time for theory γ . The time axis has been scaled by the freeze-out time as predicted by the self-similarity algorithm with respect to the correlation length, while the standard deviation has been scaled by τ_Q^β , where β is the value of the standard deviation power law exponent for theory γ , as determined by the results of the final winding statistics. The yellow shaded region indicates the impulse regime where KZM approximates the system dynamics as frozen.

may be expected since the quench removes the system from equilibrium and hence the energy-damping becomes significant. We again rescale the standard deviation by τ_Q^β with $\beta = 0.0996$, the power law exponent found numerically for the final winding standard deviation. This is shown in Figure 4.17b, where the curves now reach a universal stationary value. In contrast to the number-damping case the curves do not coincide at $t = 0$, instead displaying a region of overlap early in the quench protocol. Again, the curves seem to show some signs of self-similarity. Although rescaling the time axis did not result in a universal curve for the number-damping case, we apply the same procedure to these results regardless. The time axis is rescaled by the freeze-out time $\hat{t}$ using the value of $z\nu$ predicted by the self-similarity algorithm with respect to the correlation length ($z\nu = 2.057$). This is shown in Figure 4.18, where we see that, as was the case for theory γ the rescaling has not resulted in the curves collapsing to a universal value. In addition, the universality of the winding standard deviation near $t = 0$ that we saw from theory γ is now absent. This breakdown of universality in the impulse regime may be a sign of increasing invalidation of the adiabatic-impulse approximation, on which the derivation of KZM equations are based. However the KZM prediction of power-law behaviour has been validated by the earlier results for theory ε in subsections 4.6.1, 4.6.2, and 4.6.3, thus the particular form of universality in the impulse regime does not appear to



(a)



(b)

Figure 4.17: The winding number standard deviation over time for several values of the quench time for theory ε . In (a) the standard deviation is left unchanged while in (b) it is scaled by τ_Q^β , where β is the value of the standard deviation power law exponent for theory ε , as determined by the results of the final winding statistics.

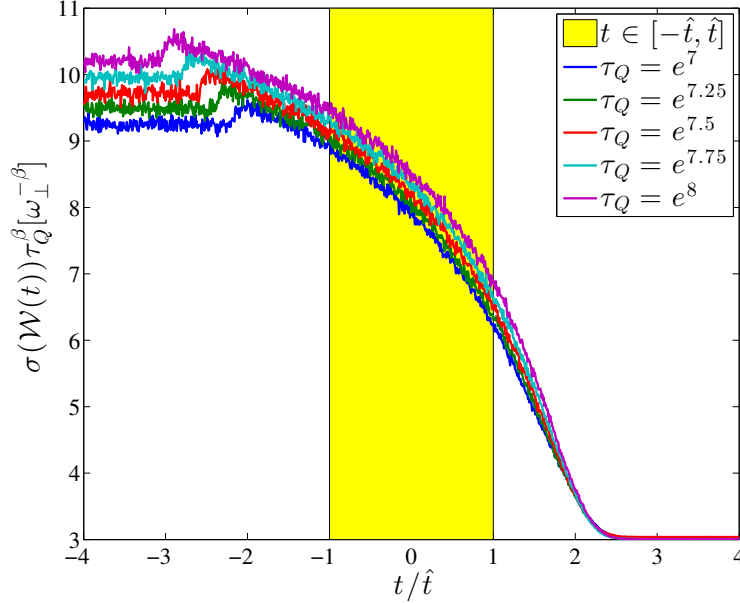


Figure 4.18: The winding number standard deviation over time for several values of the quench time for theory ε . The time axis has been scaled by the freeze-out time as predicted by the self-similarity algorithm with respect to the correlation length, while the standard deviation has been scaled by τ_Q^β where β is the value of the standard deviation power law exponent as determined by the results of the final winding statistics. The yellow shaded region indicates the impulse regime where KZM approximates the system dynamics as frozen.

be crucial to the KZM theory.

4.6.5 Rescaling Analysis of Critical Exponents

In table 4.1 we have collected the numerically obtained power law exponents resulting from our investigations, in addition to those predicted by various models. According to KZM, the critical exponents ν and z are related to the power law exponents for the freeze-out time and final winding, α and β , by equations (4.8) and (4.23) respectively. We can thus use the numerical power law exponents to obtain predictions for the critical exponents. We have one value of β , from the final winding statistics, and two values of α , from the condensate number and correlation length, for each theory, and so we will have two sets of predictions for each theory depending on which α we choose to use.

The critical exponents extracted from the results of theory γ are $\nu = 0.5064 \pm 0.0586$ and $z = 2.071 \pm 0.236$ using the value of α from the condensate number analysis, or $\nu = 0.5063 \pm 0.0772$ and $z = 2.070 \pm 0.309$ using the value of α from the correlation length analysis. These values are well within error of each other, and more importantly within error of the mean field values $\nu = 1/2$ and $z = 2$. This indicates that the number-damping sub theory of the SPGPE is a type of mean field theory, as is already known.

	Condensate Number	Correlation Length	Winding Statistics
Theory γ	$\alpha = 0.5119 \pm 0.0178$	$\alpha = 0.5118 \pm 0.0357$	$\beta = 0.1236 \pm 0.0098$
Theory ε	$\alpha = 0.7145 \pm 0.0358$	$\alpha = 0.6729 \pm 0.0364$	$\beta = 0.0966 \pm 0.0128$
Mean Field	$\alpha = 0.5$	$\alpha = 0.5$	$\beta = 0.125$
F-Model	$\alpha = 0.5$	$\alpha = 0.5$	$\beta = 0.1667$
3D XY	$\alpha = 0.5677$	$\alpha = 0.5677$	$\beta = 0.1452$
General	$\alpha = z\nu/(1 + z\nu)$	$\alpha = z\nu/(1 + z\nu)$	$\beta = \nu/2(1 + z\nu)$

Table 4.1: The power law exponents resulting from the self-similarity algorithm with respect to the condensate number and correlation length, in addition to the power law exponents found from the winding standard deviation, for both theory γ and theory ε . We have also included the values of these exponents as predicted by various universality classes.

The critical exponents extracted from the results of theory ε are $\nu = 0.6767 \pm 0.1745$ and $z = 3.698 \pm 0.675$ using the value of α from the condensate number analysis, or $\nu = 0.5906 \pm 0.1440$ and $z = 3.483 \pm 0.650$ using the value of α from the correlation length analysis. These values are distinctly different from those obtained using the results of theory γ , and though the mean field value of ν is just within error of the values of ν obtained from the results of theory ε , the value of z is not. The theory ε values of ν are also consistent with the F model [81] critical exponent $\nu = 2/3$, however the values of z are well outside the F model value $z = 3/2$, and in fact are closer to the mean field value $z = 2$. Both mean field and F model predict the product of critical exponents $z\nu = 1$, while the results of theory ε gave $z\nu = 2.503 \pm 0.439$ and $z\nu = 2.057 \pm 0.340$ using the condensate number and correlation length power-law exponent respectively. The 3D XY universality class has critical exponents $\nu = 0.6717$ and $z\nu = 1.3132$, and is thought to be the class to which the BEC transition belongs [95]. Again the values of ν are consistent with this theory while the values of z are not, however this theory predicts a larger value for $z\nu$, and thus may be considered the closest to our results. The most significant departure from the results of theory γ is the much larger values of the dynamical critical exponent z ; this may be regarded as consistent with the additional reservoir interaction terms present in theory ε .

4.7 Summary

We take this opportunity to remind the reader that in this chapter, theory γ refers to the number-damping sub-theory of the SPGPE, while theory ε refers to the full SPGPE.

To test the Kibble-Zurek mechanism, we have simulated quenches of chemical potential across the Bose-Einstein condensation transition for a range of quench times using both theory

γ and theory ε . From the simulations we extracted data on the condensate number, correlation length, and winding standard deviation. The Kibble-Zurek mechanism predicts that various aspects of these quantities are described by a power law with respect to the quench time. The condensate number and correlation length are predicted to exhibit rapid growth when leaving the impulse regime at $\hat{t}$, where $\hat{t}$ is a power law with respect to the quench time, the exponent characterised by the product of critical exponents $z\nu$. This universality property is known as self-similarity. Our results agreed with this prediction for both theory γ and theory ε , however the details of the power law differed between the theories. The power law exponents found from the results of theory γ were consistent with the mean field critical exponents $\nu = 1/2$ and $z = 2$, while the results of theory ε gave exponents which differed significantly from mean field theory.

We note that finding the numerical value of $\hat{t}$ required the use of the constants ξ_0 and τ_0 , which we have given in (4.43) and (4.44). The values of these constants were determined by finding the correlation function of theory γ in the symmetric phase prior to crossing the critical point. An approximate expression for the two point correlation function was found by neglecting interactions, and validated numerically. While these values are correct for theory γ , there is no reason why we would expect them to be correct for theory ε . In particular we would expect that τ_0 , and indeed z , should have some dependence on the energy-damping rate $\mathcal{M}$, since including energy-damping has been seen to provoke a faster evolution toward equilibrium. Thus, while we can numerically determine the scaling of $\hat{t}$ with respect to τ_Q for theory ε , we cannot currently make a sound prediction of the actual value. Thus the impulse regime shown in Figures 4.5b, 4.12b, and 4.18 may not be representative of where the regime truly lies. We have included it as a comparison to theory γ on the assumption that the difference is not too great. Finding the true values of ξ_0 and τ_0 with the inclusion of energy-damping is a possible area for future research.

Our results suggest that the dynamical critical exponent z may be an emergent quantity, i.e. not one that can be determined by universality arguments, but rather dependent on the precise reservoir interactions of a given system. To our knowledge we have given the most complete treatment of the reservoir interactions in the BEC transition, however much of the detail of a particular experiment is missing from our model, most notably the reservoir dynamics. Further work is required to determine the validity of the critical exponents that characterise the dynamical BEC transition.

The Kibble-Zurek mechanism also predicted a power law relationship between the final winding standard deviation and the quench time. We obtained the winding statistics from our quenches and found that this was indeed the case for both theory γ and theory ε . The results of theory γ gave a power law exponent consistent with mean field theory, while the results of theory ε again gave a power law exponent that differed significantly. The winding standard deviation power law exponent and the freeze-out time power law exponent were used together

to obtain numerical values of the critical exponents ν and z , with the values from theory γ being consistent with mean field theory. The values from theory ε were inconsistent with mean field, and we were unable to find a universality class with critical exponents consistent with our results, although the correlation length critical exponent ν was within error of that predicted by mean field theory, 3D XY theory, and F model theory.

Although the theory of the Kibble-Zurek mechanism did not make any predictions regarding self-similarity of the winding standard deviation over the course of quenches, both the theory γ and theory ε showed promising signs of this occurring. Upon closer inspection of Figure 4.16, the results of theory γ showed signs of universality near the transition point $t = 0$, where the winding standard deviation coincided for multiple values of the quench time. The results of theory ε did not retain this feature, with the only self-similarity being the final winding standard deviation, as was already predicted and verified. This could be indicative of a breakdown in universality caused by the inclusion of energy-damping.

Number-damping is the lowest order interaction possible between the **C**-field and the thermal reservoir, hence it should be the most significant near the transition. Higher order interactions should be less important. However the SPGPE reveals that the next order terms, describing the energy-damping interaction, can also be significant. The relative weighting of the number-damping and energy-damping terms depends strongly on how far removed the system is from equilibrium, thus driving across a phase transition is a good test of the effects of the higher order terms.

Chapter 5

Bright Soliton Arrest

5.1 Introduction

The soliton phenomena had been known long before the existence of quantum theory. In 1834 John Scott Russell observed a solitary water wave moving at a constant velocity along a canal. He noted that the wave maintained its shape for one or two miles before being lost, and called it the ‘Wave of Translation’ [96]. Moving with constant velocity and permanent form is one of the key features of solitons, along with being localised in space and interactions with other solitons resulting in only a phase shift [38]. The existence of solitons is due to the combination of dispersion and nonlinearities in a particular medium. Generally dispersion will cause a wave packet to spread out, while nonlinearities can have number of effects depending on their nature, including collapse of the wave packet. The competing effects of dispersion and nonlinearities can produce a self-reinforcing solitary wave.

Solitons appear as solutions of a large class of partial differential equations that are both dispersive and weakly nonlinear. This class of equations is useful in describing many physical systems. Light propagating in optical fibres is a well known example of such a system, and optical solitons have been both predicted [97–99] and observed in experiments [100, 101]. These included both bright solitons, localised regions of high intensity, and dark solitons, localised regions of low intensity relative to a constant background.

Another weakly nonlinear and dispersive partial differential equation of note is the Gross-Pitaevskii equation used for modelling low temperature Bose-Einstein condensates. The one dimensional Gross-Pitaevskii equation admits analytic soliton solutions, dark solitons in the case of repulsive Bose gases [42] and bright solitons in the case of attractive Bose gases [43]. In the matter wave of a Bose-Einstein condensate, dark solitons appear as a localised minimum in the density relative to a constant background, while bright solitons appear as a localised density maximum. Both dark solitons [41] and bright solitons [17] have been experimentally observed in Bose-Einstein condensates.

In this chapter we present a derivation of a stochastic differential equation for the velocity

of a bright soliton in an attractive Bose gas trapped in a one dimensional toroid and in contact with a thermal reservoir of a second component. We compare the analytical solutions of this stochastic differential equation to numerical solutions obtained by solving the energy-damping stochastic projected Gross-Pitaevskii equation (SPGPE). These solutions include those for the velocity itself, the two-time correlation function, and the steady state power spectrum.

5.2 Two-Component Systems

We wish to consider a bright soliton in a toroidally trapped one dimensional attractive Bose gas, embedded in a three dimensional thermal cloud at temperature T . Due to the attractive nature of the particle interactions, a lower energy state can be reached by particles moving from the **I**-region to the **C**-region and increasing the number of particles in the soliton. This will cause the soliton number to grow until the large **C**-field occupation invalidates the approximations of our one dimensional **C**-field theory, or the system simply collapses. Hence it is preferable to forbid particle transfer between the two regions; this will enforce a constant soliton particle number and subsequently a stable system.

The simplest model fulfilling these requirements involves a two-component mixture of Bose gases, with equal (or nearly equal) constituent masses. A commonly employed equal-mass scenario¹ involves two distinct hyperfine states of ^{87}Rb and/or ^{85}Rb [102–105], for example $|1\rangle \equiv |F=1, m_F=-1\rangle$ and $|2\rangle \equiv |F=2, m_F=1\rangle$. We wish to be in a regime where $|1\rangle$ is Bose-condensed, and has an unpopulated **I**-region in the one dimensional theory, while $|2\rangle$ is not Bose-condensed and thus has negligible **C**-field, i.e. $T_{c,2} \ll T \ll T_{c,1}$, where $T_{c,i}$ is the critical temperature for Bose-Einstein condensation of $|i\rangle$. Such a temperature window can be arranged by either taking $N_2 \ll N_1$ for similar trapping geometries, where N_i is the number of particles in state $|i\rangle$, or, for similar particle numbers, choosing $\bar{\omega}_2 \ll \bar{\omega}_1$, where $\bar{\omega}_i$ is the geometric mean of the trapping frequencies $\bar{\omega} \equiv (\omega_x \omega_y \omega_z)^{1/3}$ for state $|i\rangle$. The latter is also convenient as the trapping frequencies can then be chosen such that component $|1\rangle$ is quasi-one dimensional in nature, while $|2\rangle$ maintains three dimensional characteristics.

In practice the different magnetic sub-levels described above have very similar magnetic moments, and the magnetic traps felt by the two states may be fairly similar. More state-dependent control over the traps may be achieved by magic wavelength optical trapping techniques for two distinct atomic species [106]. In what follows we assume that the regime of a one-dimensional superfluid embedded in a three-dimensional thermal cloud of a second component can be achieved (as shown schematically in Figure 5.1), and investigate the dynamics of a bright soliton in the superfluid component. Note that the full SPGPE theory for

¹It is certainly possible to have a two-component mixture of Bose gases with *non-equal* constituent masses, however this makes calculating the energy-damping rates a more daunting prospect. Having equal (or near-equal) masses ensures the simple result for the energy-damping rate shown in this section.

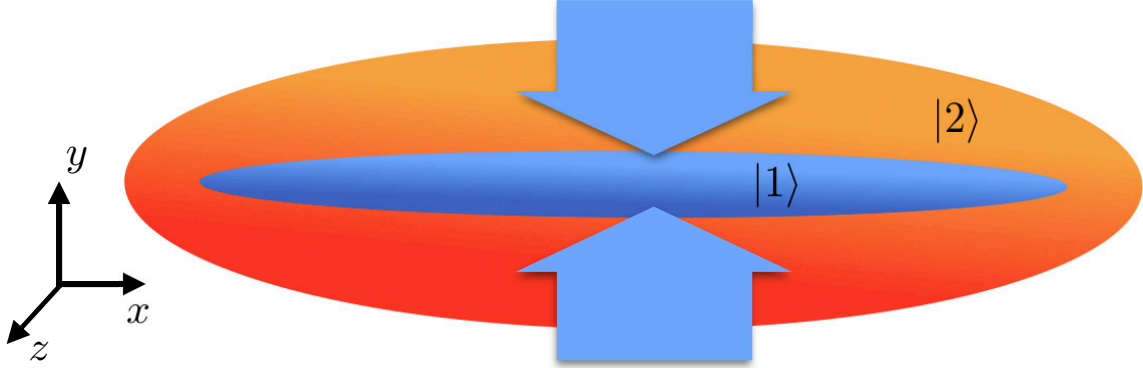


Figure 5.1: A schematic of the low-dimensional two component system. The blue represents the quasi-one dimensional Bose degenerate component $|1\rangle$ while orange represents the three dimensional thermal component $|2\rangle$. The blue arrows represent additional trapping applied to component $|1\rangle$, possibly from a blue-detuned laser, that does not affect component $|2\rangle$. The additional trapping gives the Bose degenerate component its one dimensional nature.

spinor and multicomponent systems was recently derived by Bradley and Blakie [51]. That article provides the theoretical framework for the present chapter.

We summarise the SPGPE equation of motion for $\psi_1(\mathbf{r})$ in this regime, making use of the fact that $\psi_2(\mathbf{r}) \equiv 0$, and that the **I**-region for $|1\rangle$ is unpopulated. As only one component evolves in the SPGPE theory, we will neglect the subscript denoting the component. The Hamiltonian evolution for $|1\rangle$ is

$$i\hbar d\psi_{\mathbf{C}}(x,t)\Big|_H = \mathcal{P}\{L_{\mathbf{C}}\psi_{\mathbf{C}}(x,t)dt\}, \quad (5.1)$$

where

$$L_{\mathbf{C}}\psi_{\mathbf{C}}(x,t) = (H_{\text{sp}} + g_1|\psi_{\mathbf{C}}(x,t)|^2)\psi_{\mathbf{C}}(x,t), \quad (5.2)$$

generates the projected Gross-Pitaevskii equation for Hamiltonian **C**-field evolution [12], with one dimensional interaction strength g_1 related to the s-wave scattering length a_s and transverse trapping frequency $\omega_{\perp}$ by

$$g_1 = 2\hbar\omega_{\perp}a_s. \quad (5.3)$$

Inspection of the number-damping terms shows that the rates vanish identically for the regime we consider [51]; physically this comes about as there is no population in the **I** region of the first component. Finally, a similar inspection of the energy-damping terms reveals only one contributing term, namely

$$(S)i\hbar d\psi_{\mathbf{C}}(x,t)\Big|_{\varepsilon} = \mathcal{P}\{V_{\varepsilon}(x,t)\psi_{\mathbf{C}}(x,t)dt - \hbar\psi_{\mathbf{C}}(x,t)dW_{\varepsilon}(x,t)\}, \quad (5.4)$$

where the energy-damping potential is

$$V_\varepsilon(x, t) = -\hbar \int dx' \varepsilon(x - x') \partial_{x'} j(x', t), \quad (5.5)$$

with $j(x, t)$ the one dimensional $\mathbf{C}$ -field current

$$j(x, t) = \frac{i\hbar}{2m} [\psi_{\mathbf{C}}(x, t) \partial_x \psi_{\mathbf{C}}^*(x, t) - \psi_{\mathbf{C}}^*(x, t) \partial_x \psi_{\mathbf{C}}(x, t)] \quad (5.6)$$

and the function $\varepsilon(x)$ is defined as

$$\varepsilon(x) = \frac{\mathcal{M}_{12}}{2\pi} \int dk e^{ikx} S_1(k), \quad (5.7)$$

where in general

$$\mathcal{M}_{12} = \frac{4\pi a_{12}^2}{e^{\beta(\epsilon_{\text{cut}2} - \mu_2)} - 1} \quad (5.8)$$

and a_{12} gives the s-wave interactions between the two components [51]. Here $\epsilon_{\text{cut}i}$ is the energy cutoff and μ_i is the chemical potential of component $|i\rangle$. The noise correlation is

$$\langle dW_\varepsilon(x, t) dW_\varepsilon(x', t) \rangle = \frac{2k_B T}{\hbar} \varepsilon(x - x') dt, \quad (5.9)$$

and the one-dimensional scattering kernel is defined by

$$S_1(k) = \sqrt{\frac{\eta}{8\pi}} G\left(\frac{|k|}{\sqrt{2\eta}}\right) \quad (5.10)$$

with η related to the transverse harmonic trapping frequency $\omega_\perp$ or width $a_\perp$ by

$$\eta = \frac{m\omega_\perp}{\hbar} = \frac{1}{a_\perp^2}. \quad (5.11)$$

At this point we wish to emphasise that we have identified a regime where the number-damping terms are absent, and the only energy terms are between a condensed component $|1\rangle$ and a non-condensed component $|2\rangle$. The strength of the energy-damping, $\mathcal{M}_{12}$, is determined by the inter-component scattering length, and by the population of component $|2\rangle$ at the cutoff energy $\epsilon_{\text{cut}2}$. While it appears to only depend on the population at the cutoff, this term is the result of a collision integral that accounts for all of the energy-damping collisions due to $|2\rangle$ atoms with energy exceeding $\epsilon_{\text{cut}2}$. Since $T > T_{c,2}$, $\mu_2 < 0$, and to a first approximation we can take $\epsilon_{\text{cut}2} \simeq 0$, including all of component $|2\rangle$ in the reservoir for $|1\rangle$ gives the energy-damping

rate

$$\mathcal{M}_{12} = \frac{4\pi a_{12}^2}{e^{\beta|\mu_2|} - 1}. \quad (5.12)$$

This energy-damping rate differs from the single-component energy-damping rate (3.71) by a factor of four. This is due to the particles in the **C**-field and **I**-field being indistinguishable for the single-component system, but distinguishable for the two-component system. A factor of 4 appears, rather the usual factor of 2, due to the fact that the energy damping process incorporates both forward and backward processes into a single rate function, and a factor of 2 occurs for each of these distinct scattering channels.

5.3 Soliton Projection

Our system of a bright soliton in a toroidally trapped one dimensional attractive Bose gas, embedded in a three dimensional thermal cloud of temperature T , is appropriately modelled by the energy-damping SPGPE

$$(S)d\psi_{\mathbf{C}}(x, t) = d\psi_{\mathbf{C}}(x, t)\Big|_H + (S)d\psi_{\mathbf{C}}(x, t)\Big|_{\varepsilon} \quad (5.13)$$

where the two terms are given by (5.1) and (5.4) from the preceding section. Because we are considering an attractive gas, the s-wave scattering length a_s is negative. Since there is only one damping rate present in the problem, we drop the subscript from the energy-damping rate, setting

$$\mathcal{M} \equiv \mathcal{M}_{12}. \quad (5.14)$$

The bright soliton analytic solution of the one dimensional Gross-Pitaevskii equation is

$$\phi_s(x, t) = \sqrt{\frac{N}{2\kappa}} \operatorname{sech}\left(\frac{x - x(t)}{\kappa}\right) \exp\left[\frac{imv}{\hbar}x + \frac{i}{\hbar}\left(\frac{mv^2}{2} - \frac{\hbar^2}{2m\kappa}\right)t\right] \quad (5.15)$$

where $x(t)$ is the location of the soliton center of mass and $v \equiv \dot{x}(t)$ is the soliton velocity. From (5.15) it is clear that the superfluid velocity

$$v_s(x) \equiv \frac{\hbar}{m}\partial_x\Theta(x), \quad (5.16)$$

where $\Theta(x)$ is the superfluid phase, is spatially invariant and equal to the soliton velocity

$$v_s(x) \equiv v. \quad (5.17)$$

The soliton particle number N and the soliton width κ are related by

$$N = \frac{2\hbar^2}{m|g_1|\kappa}, \quad (5.18)$$

hence increasing the particle number results in a more spatially localised soliton. The energy per particle of the bright soliton solution is

$$\frac{E}{N} = \frac{mv^2}{2} - \frac{\hbar^2}{6m\kappa^2}, \quad (5.19)$$

from which we see that increasing the particle number N , and thus decreasing the soliton width κ , results in a lower energy state. Our goal is to reduce the energy-damping SPGPE (5.13) to an equivalent stochastic differential equation for the soliton velocity v .

5.3.1 Ito SPGPE

To make the change of variables, we need to first write (5.13) in the Ito form, so that the noise $dW_\varepsilon(x, t)$ and wave function $\psi_{\mathbf{C}}(x, t)$ are uncorrelated. The Fokker-Planck equation that maps to (5.13) is

$$\begin{aligned} \frac{\partial W_{\mathbf{C}}}{\partial t} = & \int dx \left[-\frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x)} \left(-\frac{i}{\hbar} L_{\mathbf{C}}\psi_{\mathbf{C}}(x) - \frac{i}{\hbar} V_\varepsilon(x, t)\psi_{\mathbf{C}}(x) \right) + \text{h.c.} \right] W_{\mathbf{C}} \\ & + \int dx \int dx' \left[\frac{k_B T}{\hbar} \varepsilon(x - x') \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x)} \psi_{\mathbf{C}}(x) \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}^*(x')} \psi_{\mathbf{C}}^*(x') + \text{h.c.} \right] W_{\mathbf{C}} \\ & - \int dx \int dx' \left[\frac{k_B T}{\hbar} \varepsilon(x - x') \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x)} \psi_{\mathbf{C}}(x) \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x')} \psi_{\mathbf{C}}(x') + \text{h.c.} \right] W_{\mathbf{C}}. \end{aligned} \quad (5.20)$$

To map to an Ito form, the derivatives in (5.20) must be rearranged [107]. This is done by using

$$\frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x')} (\psi_{\mathbf{C}}(x) W_{\mathbf{C}}) = \left(\psi_{\mathbf{C}}(x) \frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x')} + \delta(x, x') \right) W_{\mathbf{C}}. \quad (5.21)$$

The resulting equation is

$$\begin{aligned} \frac{\partial W_{\mathbf{C}}}{\partial t} = & \int dx \left[-\frac{\bar{\delta}}{\bar{\delta}\psi_{\mathbf{C}}(x)} \mathcal{L}_D \psi_{\mathbf{C}}(x) + \text{h.c.} \right] W_{\mathbf{C}} \\ & + \int dx \int dx' \left[\frac{k_B T}{\hbar} \varepsilon(x - x') \frac{\bar{\delta}^{(2)}}{\bar{\delta}\psi_{\mathbf{C}}(x) \bar{\delta}\psi_{\mathbf{C}}^*(x')} \psi_{\mathbf{C}}(x) \psi_{\mathbf{C}}^*(x') + \text{h.c.} \right] W_{\mathbf{C}} \\ & - \int dx \int dx' \left[\frac{k_B T}{\hbar} \varepsilon(x - x') \frac{\bar{\delta}^{(2)}}{\bar{\delta}\psi_{\mathbf{C}}(x) \bar{\delta}\psi_{\mathbf{C}}(x')} \psi_{\mathbf{C}}(x) \psi_{\mathbf{C}}(x') + \text{h.c.} \right] W_{\mathbf{C}}. \end{aligned} \quad (5.22)$$

where we have defined the operator

$$\mathcal{L}_D \psi_{\mathbf{C}}(x) = \left[-\frac{i}{\hbar} L_{\mathbf{C}} - \frac{i}{\hbar} V_{\varepsilon}(x, t) - \frac{k_B T}{\hbar} \varepsilon(0) \right] \psi_{\mathbf{C}}(x) \quad (5.23)$$

and we introduce the shorthand

$$\varepsilon(0) \psi_{\mathbf{C}}(x) \equiv \int dx' \varepsilon(x - x') \delta_{\mathbf{C}}(x, x') \psi_{\mathbf{C}}(x'). \quad (5.24)$$

We can now map this to an Ito projected stochastic differential equation

$$d\psi_{\mathbf{C}} = \mathcal{P} \{ \mathcal{L}_D \psi_{\mathbf{C}} dt + i\psi_{\mathbf{C}} dW_{\varepsilon}(x, t) \}. \quad (5.25)$$

5.3.2 Change of Variables

The momentum of any system can be found using

$$P[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*] = \frac{i\hbar}{2} \int dx [\psi_{\mathbf{C}}(x) \partial_x \psi_{\mathbf{C}}^*(x) - \psi_{\mathbf{C}}^*(x) \partial_x \psi_{\mathbf{C}}(x)], \quad (5.26)$$

a functional with respect to $\psi_{\mathbf{C}}$ and $\psi_{\mathbf{C}}^*$. If we compare this to the particle density current $j(x)$

$$j(x) = \frac{i\hbar}{2m} [\psi_{\mathbf{C}}(x) \partial_x \psi_{\mathbf{C}}^*(x) - \psi_{\mathbf{C}}^*(x) \partial_x \psi_{\mathbf{C}}(x)], \quad (5.27)$$

we see that

$$P[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*] = m \int dx j(x). \quad (5.28)$$

Also, we may define the particle density current as

$$j(x) = n(x)v \quad (5.29)$$

where $n(x)$ is the particle density and v is the velocity, which is spatially invariant. Hence we see that the velocity and momentum are related in the classical sense

$$P = Nmv \quad (5.30)$$

and we can thus define the velocity functional

$$v[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*] = \frac{i\hbar}{2Nm} \int dx [\psi_{\mathbf{C}}(x) \partial_x \psi_{\mathbf{C}}^*(x) - \psi_{\mathbf{C}}^*(x) \partial_x \psi_{\mathbf{C}}(x)]. \quad (5.31)$$

This also encourages us to consider the bright soliton as a quasiparticle of mass Nm and velocity v . The Ito rule for change of variables [107] now takes the form

$$\begin{aligned} dv[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*] &= \int dx \frac{\bar{\delta}v[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*]}{\bar{\delta}\psi_{\mathbf{C}}(x)} d\psi_{\mathbf{C}}(x) + \text{h.c.} \\ &+ \frac{k_B T}{\hbar} \int dx \int dx' \frac{\bar{\delta}^{(2)}v[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*]}{\bar{\delta}\psi_{\mathbf{C}}(x)\bar{\delta}\psi_{\mathbf{C}}^*(x')} \psi_{\mathbf{C}}(x)\psi_{\mathbf{C}}^*(x')\varepsilon(x-x')dt + \text{h.c.} \\ &- \frac{k_B T}{\hbar} \int dx \int dx' \frac{\bar{\delta}^{(2)}v[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*]}{\bar{\delta}\psi_{\mathbf{C}}(x)\bar{\delta}\psi_{\mathbf{C}}(x')} \psi_{\mathbf{C}}(x)\psi_{\mathbf{C}}(x')\varepsilon(x-x')dt + \text{h.c.} \end{aligned} \quad (5.32)$$

up to order dt . The velocity functional (5.31) has the first functional derivative

$$\frac{\bar{\delta}v}{\bar{\delta}\psi_{\mathbf{C}}(x)} = \frac{i\hbar}{Nm} \mathcal{P}^* \{ \partial_x \psi_{\mathbf{C}}^*(x) \} \quad (5.33)$$

while one of the two required second functional derivatives vanishes

$$\frac{\bar{\delta}^{(2)}v}{\bar{\delta}\psi_{\mathbf{C}}(x)\bar{\delta}\psi_{\mathbf{C}}(x')} = 0, \quad (5.34)$$

$$\frac{\bar{\delta}^{(2)}v}{\bar{\delta}\psi_{\mathbf{C}}(x)\bar{\delta}\psi_{\mathbf{C}}^*(x')} = \frac{i\hbar}{Nm} \mathcal{P}^* \{ \partial_x \delta(x, x') \}. \quad (5.35)$$

These relied on the fact that $dN = 0$ and thus N is constant; in general $N[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*]$ is a functional, and the functional derivatives of $v[\psi_{\mathbf{C}}, \psi_{\mathbf{C}}^*]$ would then differ. Evaluating the change of variables using the soliton wave function (5.15) and neglecting the projectors gives the stochastic differential equation

$$dv = -\Lambda_s v dt + \sqrt{\beta} dW(t) \quad (5.36)$$

where

$$\Lambda_s \equiv \hbar \mathcal{M} \frac{4N}{m\pi^4 \kappa^3} \sqrt{\frac{\eta}{8\pi}} \mathcal{I}_1 \quad (5.37)$$

is the decay rate,

$$\beta \equiv \hbar \mathcal{M} \frac{8k_B T}{m^2 \pi^4 \kappa^3} \sqrt{\frac{\eta}{8\pi}} \mathcal{I}_1, \quad (5.38)$$

is the diffusion constant, and the integral

$$\mathcal{I}_1 \equiv \int_{-\infty}^{\infty} dx G \left(\sqrt{\frac{2}{\eta \pi \kappa}} |x| \right) x^4 \text{csch}^2(x), \quad (5.39)$$

with $G(x) \equiv e^{x^2} \operatorname{erfc}(x)$ the scaled complementary error function and $\operatorname{csch}(x) \equiv 2/(e^x - e^{-x})$ the hyperbolic cosecant, has some geometry dependence. Note that (5.37), (5.38) and (5.39) are all time-independent. The noise $dW(t)$ is a Wiener process with unit correlation

$$\langle dW(t)dW(t') \rangle = dt. \quad (5.40)$$

Note that the Stratonovich correction present in (5.23) does not appear in the final equation of motion. It turns out that the contribution from non-zero second derivative term of (5.32) gives a term that precisely cancels with the term arising due to the Stratonovich correction. Neglecting the noise briefly, equation (5.36) is equivalent to having the soliton quasi-particle subjected to a frictional force $F = -Nm\Lambda_s v$ in the small velocity limit. In [108] a frictional force on a matter wave bright soliton was derived due to an extra nonlinearity arising due to deviations from the quasi-one-dimensional limit, while here the frictional force is a consequence of interaction with the incoherent thermal field.

5.3.3 Analytic Solutions

Equation (5.36) is in the form of an Ornstein-Uhlenbeck process, the solutions of which are well-known [107]. The velocity is given by

$$v(t) = v_0 e^{-\Lambda_s t} + \sqrt{\beta} \int_0^t e^{-\Lambda_s(t-t')} dW(t') \quad (5.41)$$

where v_0 is the initial soliton velocity. The steady-state variance of the velocity is

$$\lim_{t \rightarrow \infty} \langle v^2 \rangle = \frac{\beta}{2\Lambda_s} = \frac{k_B T}{Nm} \quad (5.42)$$

which is equivalent to a statement of the equipartition theorem for a particle of mass Nm in an ideal thermal gas of temperature T in one dimension. The two-time correlation function of the soliton velocity is

$$\langle v(t)v(t') \rangle = \left(v_0^2 - \frac{k_B T}{Nm} \right) e^{-\Lambda_s(t+t')} + \frac{k_B T}{Nm} e^{-\Lambda_s|t-t'|} \quad (5.43)$$

which reduces in the steady-state limit to

$$\lim_{t, t' \rightarrow \infty} \langle v(t)v(t') \rangle = \frac{k_B T}{Nm} e^{-\Lambda_s|t-t'|} = G(\tau), \quad (5.44)$$

dependent only on the single variable $\tau = t - t'$. The Wiener-Khinchin theorem [109, 110] states that the two-time correlation function and spectrum of a quantity are a Fourier transform

pair

$$S(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega\tau} G(\tau) d\tau, \quad G(\tau) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega\tau} S(\omega) d\omega \quad (5.45)$$

and thus the velocity spectrum is

$$S(\omega) = \sqrt{\frac{2}{\pi}} \frac{k_B T}{Nm} \frac{\Lambda_s}{\omega^2 + \Lambda_s^2}. \quad (5.46)$$

These solutions are also equivalent to the Brownian motion of a particle of mass Nm immersed in a thermal environment of temperature T . Thus the quantum Brownian motion of a bright soliton, described by the energy-damping SPGPE, reduces to an equation resembling classical Brownian motion for the soliton center of mass.

5.4 Numerical Procedure

We simulate evolution of a one dimensional toroidally trapped attractive Bose gas with the initial value of the $\mathbf{C}$ -field wave function given by the analytic bright soliton solution (5.15) at $t = 0$. The simulations are performed by numerically solving the energy-damping stochastic projected Gross-Pitaevskii equation (5.13). Our goal is to determine if these numerical solutions are consistent with the solutions of the soliton velocity stochastic differential equation (5.36) derived in the preceding section.

5.4.1 Dimensionless Units

Our system consists of a a quasi-one dimensional toroid with harmonic transverse trapping characterised by a trapping frequency of $\omega_{\perp}/2\pi = 200\text{Hz}$. This parameter then defines our system of dimensionless units

$$x_0 = a_{\perp} = \sqrt{\frac{\hbar}{m\omega_{\perp}}}, \quad t_0 = \frac{ma_{\perp}^2}{\hbar} = \frac{1}{\omega_{\perp}}, \quad E_0 = \frac{\hbar^2}{ma_{\perp}^2} = \hbar\omega_{\perp}.$$

We could also have chosen the dimensionless units to be based around the system length L , or the healing length of the gas. The chosen system of units is convenient as it results in the length L of the system also being the anisotropy.

5.4.2 Simulation Parameters

We use parameters consistent with the atomic species lithium-7, commonly used in experiments involving Bose-Einstein condensation of attractive gases. These parameters include the mass $m = 7u$, where u is the atomic mass unit, and the s-wave scattering length $a_s = -5a_0$ where a_0 is the Bohr radius. A range of scattering lengths can be accessed experimentally in lithium-7 by utilising a Feshbach resonance [40]. Both these parameters along with the transverse trapping frequency, are used in determining the interaction parameter $g_1 = 2\hbar\omega_\perp a_s$. The chosen parameters result in the value of the one dimensional interaction parameter being $g_1 = -1.97 \times 10^{-4} \hbar\omega_\perp a_\perp$.

We consider a system of length $L = 50a_\perp$ simulated on a grid consisting of $M = 1024$ points with periodic boundary conditions. A realistic value for the damping rates in experiments involving dynamics is $\mathcal{O}(10^{-4})$ (see e.g. [4]), thus we use a constant dimensionless energy-damping rate of $\mathcal{M} = 10^{-4}$. The initial soliton wave function has a width of $\kappa = a_\perp$. This results in a soliton containing $N \approx 10,000$ particles. In [111] a bright soliton containing $N \approx 6000$ particles was observed, while in [112] pairs of bright solitons containing $N \approx 28000$ particles were created for studying collisions; our particle number falls in between these experimentally accessible values. The ratio $\kappa/L = 0.02$ is small enough such that the soliton evolves as if it were in an infinitely long spatial domain, despite the periodicity of the system.

The temperature is held constant at $T = 0.5T_c$ where T_c is the transition temperature for the ideal Bose gas in a box potential of length L , embedded in a 3D thermal cloud where the two tightly confined directions are harmonically trapped. It can be shown [89] that this critical temperature is given by

$$T_c = \frac{\hbar\bar{\omega}}{k_B} \left(\frac{N}{\zeta(5/2)} \right)^{2/5} \quad (5.47)$$

with $\bar{\omega}$ the modified geometric mean frequency

$$\bar{\omega}^5 = \frac{2\pi\hbar}{mL^2} \omega_\perp^4, \quad (5.48)$$

and N the particle number. To calculate the critical temperature T_c we have used for N the number of particles contained in the soliton.

The energy-damping SPGPE is solved numerically using a weak semi-implicit Euler method, the details of which can be found in [7, 65]. The initial wave function is given by (5.15) with $t = 0$. The time step we use in our simulations is $dt = 0.0005\omega_\perp^{-1}$, much smaller than any other time scale involved in the system evolution, and we evolve the system for a total time $t = 300\omega_\perp^{-1}$. The theory contains noise, thus we need to take ensemble averages to obtain meaningful results. Each set of 500 trajectories took ~ 90 hours to simulate, due to the slowly converging weak semi-implicit Euler algorithm.

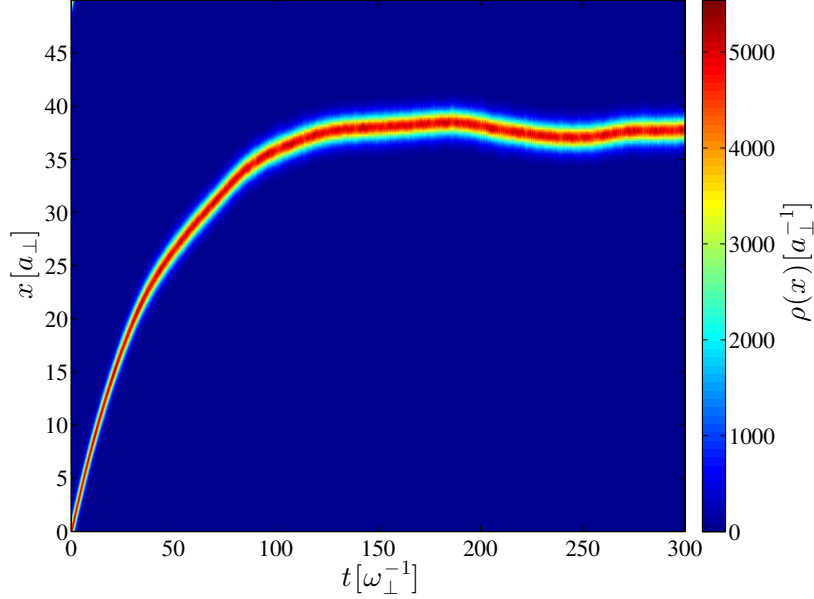


Figure 5.2: Particle density over time for one soliton trajectory with an initial position $x = 0$ and initial velocity $v_0 = 0.9a_\perp\omega_\perp$.

5.5 Results

In this section we present the various results we have obtained from simulating the motion of a bright soliton in our system. For each piece of data we will mention the method by which it was obtained and how it compares to the solutions of (5.36). An example of a typical trajectory for a bright soliton with initial velocity $v_0 = 0.9a_\perp\omega_\perp$ is shown in Figure 5.2. The position over time appears exponential, indicating the soliton experiences a retarding force proportional to its instantaneous velocity. After some time the varying position of the soliton position appears to fluctuate around a constant value. In Figure 5.3 we show how the particle density has changed after evolving the initial stationary soliton wave function for $t = 300\omega_\perp^{-1}$ using the energy-damping SPGPE. This shows that the functional form has changed very little, with the wave function developing some small fluctuations in addition to a slight translation. This justifies our assumption that the soliton maintains its functional form during evolution.

5.5.1 Velocity

We test the prediction (5.41) for an ensemble of trajectories. The average velocity over a large number of trajectories is given by

$$\langle v(t) \rangle = v_0^2 e^{-\Lambda_s t}. \quad (5.49)$$

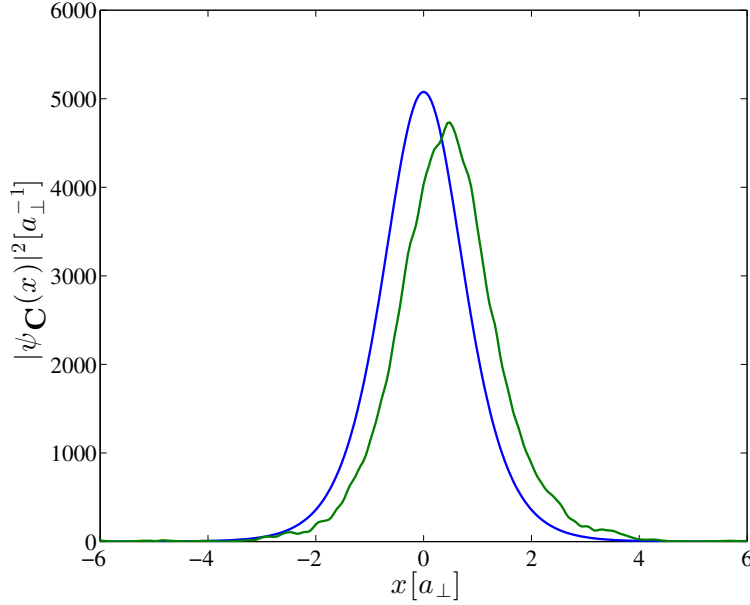


Figure 5.3: Particle density at $t = 0$ (blue) and $t = 300\omega_{\perp}^{-1}$ (green) for an initially stationary bright soliton. The initial wave function is given by (5.15), with further evolution simulated using the energy-damping SPGPE.

The numerical velocity for any one trajectory is found by evaluating the expectation value

$$v(t) = \frac{1}{Nm} \int dx \psi_{\mathbf{C}}^*(x, t) (-i\hbar \partial_x) \psi_{\mathbf{C}}(x, t) \quad (5.50)$$

of the numerically obtained wave function $\psi_{\mathbf{C}}(x, t)$. The average velocity is then simply the ensemble average

$$\langle v(t) \rangle = \left\langle \frac{1}{Nm} \int dx \psi_{\mathbf{C}}^*(x, t) (-i\hbar \partial_x) \psi_{\mathbf{C}}(x, t) \right\rangle. \quad (5.51)$$

In Figure 5.4 we show the average velocity over time for a bright soliton with initial velocity $v_0 = 0.9a_{\perp}\omega_{\perp}$. The numerical data from 500 trajectories compares very well with the analytic expression arising from the solution of (5.36), exhibiting exponential decay with the characteristic decay constant Λ_s .

We also look at the variance of the velocity over time. From (5.49) and (5.43) it is trivial to show that

$$\sigma^2(v(t)) = \frac{k_B T}{Nm} (1 - e^{-2\Lambda_s t}) \quad (5.52)$$

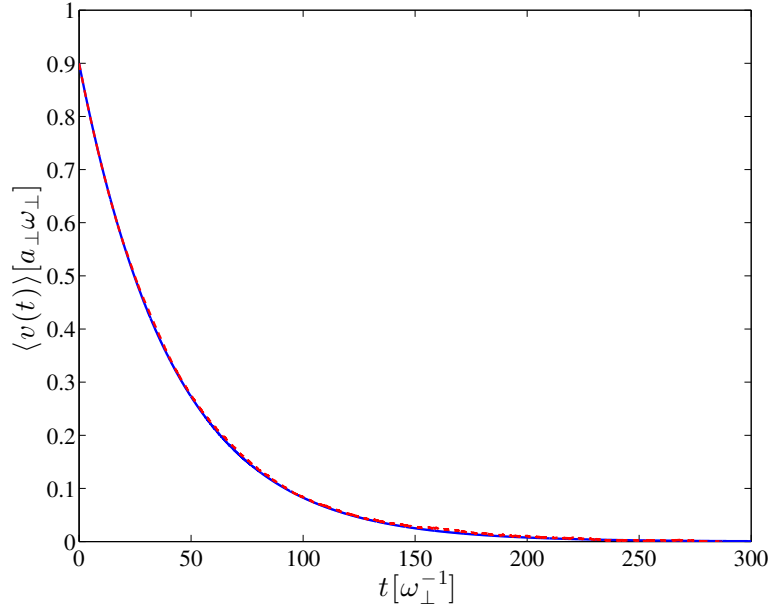


Figure 5.4: Average soliton velocity over time for 5000 trajectories with an initial position $x = 0$ and initial velocity $v_0 = 0.9a_{\perp}\omega_{\perp}$. The solid blue line is the analytic expression (5.49), while the dashed red line gives the numerical solution obtained via (5.51)

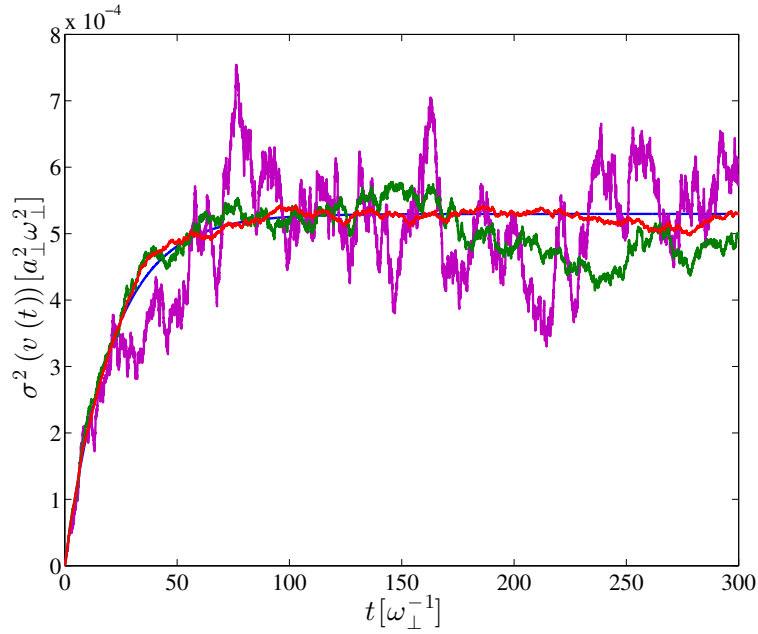


Figure 5.5: The variance of the soliton velocity over time for 50 (magenta), 500 (green), and 5000 (red) trajectories with an initial position $x = 0$ and initial velocity $v_0 = 0.9a_{\perp}\omega_{\perp}$. The blue line is the analytic expression (5.52), while the numerical values are obtained via (5.54).

where the variance σ^2 is defined by

$$\sigma^2(A) \equiv \langle A^2 \rangle - \langle A \rangle^2. \quad (5.53)$$

The ensemble of numerically obtained velocities also gives us our numerical variance

$$\sigma^2(v(t)) = \sigma^2 \left(\frac{1}{Nm} \int dx \psi_{\mathbf{C}}^*(x, t) (-i\hbar \partial_x) \psi_{\mathbf{C}}(x, t) \right). \quad (5.54)$$

In Figure 5.5 we show the standard deviation of velocity over time for 50, 500, and 5000 trajectories of a bright soliton with initial velocity $v_0 = 0.9a_{\perp}\omega_{\perp}$. The initial condition has a deterministic velocity and no noise, thus the initial standard deviation is zero. For the analytic expression the standard deviation then grows before plateauing at a constant value (5.42) as the soliton and environment reach thermal equilibrium. For early times, up to $t \approx 25\omega_{\perp}^{-1}$, the numerical data agrees well with the analytic expression for all three ensembles. After this point the numerical value exhibits fluctuations about the analytic value, with the larger ensembles showing less deviation than the smaller ensembles. These fluctuations are evidently the result of taking a finite number of trajectories, being significantly larger for the ensemble containing only 50 trajectories than the ensemble containing 5000 trajectories. The fluctuations are far more evident here than in Figure 5.4 since the standard deviation of the velocity is much smaller than the average velocity. Increasing the number of trajectories reduces the fluctuations, and we conclude that our numerical data is consistent with the analytic solution.

5.5.2 Correlations

We investigate the steady-state two-time correlation function of the soliton velocity. From Figure 5.4 we can see that for a soliton with initial velocity $v_0 = 0.9a_{\perp}\omega_{\perp}$, our parameters result in the steady state being reached after $t \approx 250\omega_{\perp}^{-1}$, leaving only $t \approx 50\omega_{\perp}$ remaining to investigate the steady-state properties. Thus instead of using the ensemble of 5000 velocity trajectories we obtained earlier, we simulate a new ensemble of 500 trajectories of an initially stationary soliton, $v_0 = 0$. The steady-state is then reached when the velocity variance reaches a constant value. The variance is independent of initial velocity, so the analytic expression (5.52) still applies. We identify the time at which the system has reached a steady state; inspection of Figure 5.5 suggests $t = 120\omega_{\perp}^{-1}$ is sufficient, thus we truncate the trajectories such that they begin at $t = 120\omega_{\perp}^{-1}$. This leaves $t = 180\omega_{\perp}^{-1}$ to investigate the steady-state properties, corresponding to approximately 4 damping times ($t \approx 4\Lambda_s^{-1}$).

The numerically obtained trajectories can be represented as a row vector of functions $\mathbf{v}(t) = [v_i(t)]$, where the index i indicates the i th trajectory. The two-time correlation function

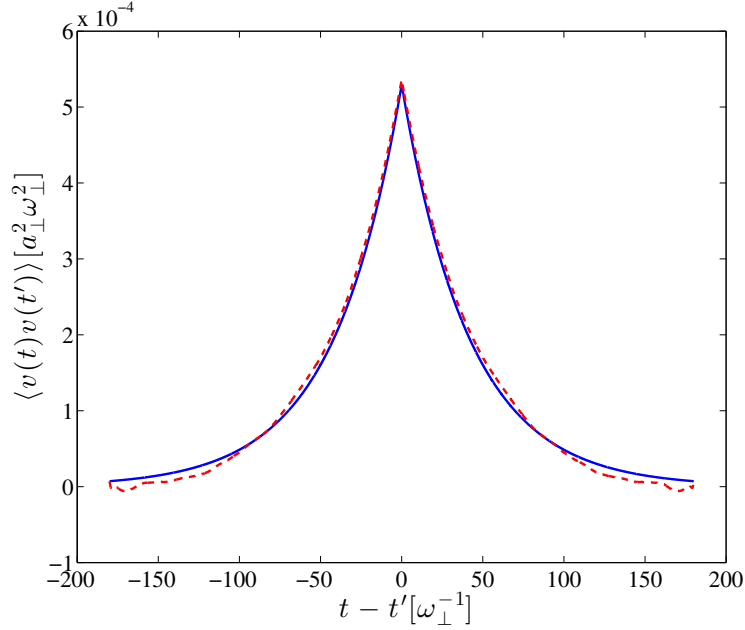


Figure 5.6: The steady-state two-time correlation function of the soliton velocity constructed using 500 trajectories of an initially stationary soliton at $x = 0$. The solid blue line is the analytic expression (5.43), while the dashed red line shows the numerically obtained values.

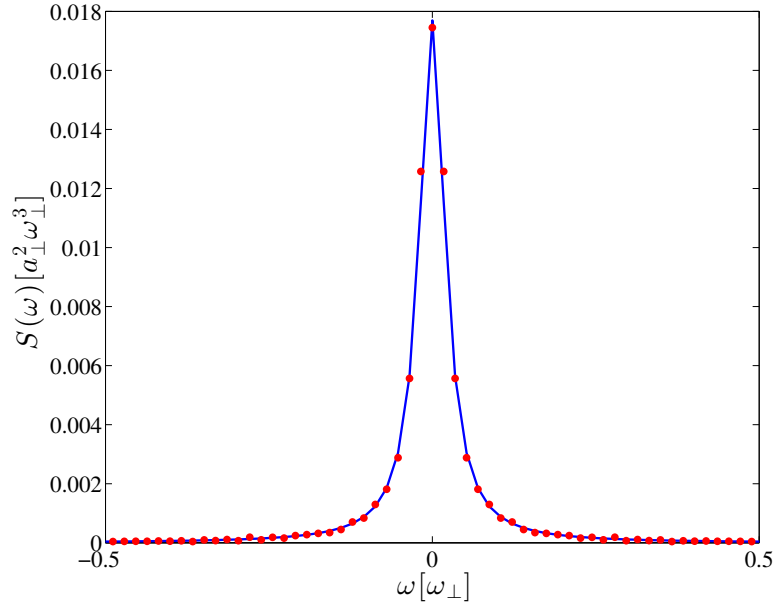


Figure 5.7: The spectrum of the soliton velocity constructed using 500 trajectories of an initially stationary soliton at $x = 0$. The solid blue line is the analytic expression (5.46), while the red points are the numerically obtained values.

is then constructed via the operation

$$\langle v(t)v(t') \rangle = \mathbf{v}(t)\mathbf{v}^T(t') = \sum_i v_i(t)v_i(t'). \quad (5.55)$$

In the steady state, the two-time correlation function should depend only on the difference between the two-time arguments t and t' . This being the case, we take the average of the values the function takes for each constant $\tau = t - t'$, obtaining a function of the single variable τ . The two-time correlation function found in this way is shown in Figure 5.6, as well as the analytic expression (5.43). We see that the numeric and analytic two-time correlation functions agree very well, with the edges of the window showing slightly less agreement. This is an artefact of averaging across the diagonal of (5.55); for every t there is a t' such that $t - t' = 0$, hence there are many data points to average over, while there is only one pair of t and t' such that $t - t' = 180\omega_{\perp}^{-1}$, and thus only one data point to average over.

Having found the two-time correlation we can also construct the velocity spectrum by exploiting the Wiener-Khinchin theorem; we simply take the Fourier transform of the numerically found correlation function. Figure 5.7 shows the velocity spectrum obtained by taking the Fourier transform of the numeric correlation function shown in Figure 5.6. Here we have excellent agreement between the analytic expression and the numerically obtained data.

5.6 Summary

We have derived a stochastic differential equation for the velocity of a bright soliton embedded in a thermal cloud of a second component. The system is described by the energy-damping stochastic projected Gross-Pitaevskii equation [51]. The resulting equation describes Brownian motion of the bright soliton quasi-particle, a type of Ornstein-Uhlenbeck process. The solutions of this equation are well known, and hence we found analytic expressions for the soliton velocity, the two-time correlation function of the velocity, and the velocity spectrum.

The simplicity of the soliton velocity solutions suggests a possible application to experiments. If one can measure the decay rate constant Λ_s , given in (5.37) and the diffusion constant β , given in (5.38), then the ratio of the two constants along with the system temperature and particle mass totally determines the number of particles in the soliton (5.42). This result could be used to determine the number of particles contained in a bright soliton experimentally.

To validate our analytical treatment, we simulated motion of a bright soliton in a one dimensional attractive Bose gas confined in a toroid by numerically solving the energy-damping stochastic projected Gross-Pitaevskii equation. Repeating for 500 trajectories we extracted an ensemble of trajectories for the soliton velocity from the $\mathbf{C}$ -field wave function using the standard method of operator expectations and the assumption that the soliton maintained

a permanent functional form. From this ensemble we constructed numerical values for the two-time correlation function and the velocity spectrum, as well as the mean and standard deviation of the velocity over time. These results were compared with the analytic solutions of the derived stochastic differential equation, and were found to show excellent agreement, providing validation of our effective stochastic differential equation. Further investigations may involve relaxing the assumption of a constant solitonic solution to probe the validity of this procedure.

The success of this method for obtaining equations for the soliton velocity suggests that we may look for applicability of the method elsewhere. An equivalent procedure can be found for the full stochastic projected Gross-Pitaevskii equation, and Ito's rule ensures that an effective stochastic differential equation may be found for any parameter provided it can be written as a functional of $\psi_{\mathbf{C}}$ and $\psi_{\mathbf{C}}^*$. The analytical tractability of the resulting equation will presumably depend on the system in question. In our case, the bright soliton evolution could be described by a single parameter, the velocity. As a contrast, the dark soliton evolution requires several time-dependent parameters, thus presumably resulting in a more complex system of stochastic differential equations.

Chapter 6

Conclusions

6.1 Thesis Summary

The modelling of finite-temperature non-equilibrium dynamics of ultra-cold Bose gases is a problem that has permeated the field. A powerful tool to approach this challenge had been developed in the form of the stochastic projected Gross-Pitaevskii equation (SPGPE), a grand canonical $\mathbf{C}$ -field theory. Investigations showed that the outcome of experiments involving Bose-Einstein condensate dynamics [2, 15] could be predicted quantitatively using this theoretical framework [3, 4], with little or no use of fitting parameters. These and other applications of the SPGPE have generally employed a sub-theory where number-conserving scattering processes, known as energy-damping, are neglected; the number-damping (or simple growth) SPGPE. The remaining processes that do not conserve number are known as number-damping. In this thesis we have used the one-dimensional SPGPE to model two possible processes in an ultra-cold gas at finite temperature. The first is quenching the chemical potential of a repulsive Bose gas across the Bose-Einstein condensation transition as a test of the Kibble-Zurek mechanism, for which we investigate the effects of including energy-damping. The second is bright soliton arrest in an attractive Bose gas, for which energy-damping was the only physically allowed reservoir interaction between the $\mathbf{C}$ -field and a thermal cloud consisting of a second component.

We modelled the quench of chemical potential of a repulsive Bose gas confined to a toroid across the Bose-Einstein condensation transition using both the full SPGPE and the number-damping sub-theory. In particular we determined the statistics for the final winding values around the toroid, as well as the growth curves of condensate number and correlation length over the course of the quenches. For the full SPGPE simulations, we set the damping rates such that the energy-damping and number-damping were approximately equally weighted; in experiments the energy-damping and number-damping rates are of similar magnitude, and we chose them to be equal. We found that the predictions of the Kibble-Zurek mechanism concerning the existence of power laws were consistent with our results, for both the full

theory and the number-damping sub-theory. The predictions of the power law exponents are determined by the critical exponents of the transition, themselves determined by the universality class. Our results for the number-damping sub-theory agreed with the predictions of mean field theory, a finding that has been previously reported [50, 79]. The full SPGPE departed from mean field theory for the dynamical critical exponent, and we were unable to find a universality class with critical exponents consistent with our findings. The departure from mean field of these results may be considered to be our most significant result, as the Bose-Einstein condensation transition is not believed to be described by mean field exponents, but rather to be in the 3D XY model universality class [95]. While our full SPGPE results were not consistent with this universality class either, there is still the question of relative weights for the two damping processes, which may have an effect on the critical exponents. The difference lies in the dynamical critical exponent, consistent with our inclusion of an additional damping process in our simulations of the transition.

We then applied the SPGPE to the motion of a bright soliton in an attractive Bose gas in contact with a thermal cloud of a second component. For this we used a form of the SPGPE which only included the number-conserving scattering processes, known as the energy-damping SPGPE. In an attractive Bose gas, the presence of non-number-conserving processes would cause particles to move from the thermal cloud to $\mathbf{C}$ -field until the system collapsed. We found a procedure using the Ito calculus to change variables from an equation describing time evolution of the $\mathbf{C}$ -field wave function to an equation describing time evolution of the soliton velocity, which took the form of an Ornstein-Uhlenbeck process. This procedure could be extended to the full SPGPE and applied to any system where the wave function is able to be described by a small set of parameters. We simulated the motion of bright solitons with an initial non-zero velocity using the energy-damping SPGPE and compared these results with the analytic solutions of the velocity stochastic differential equation. These showed excellent agreement, thus validating our equation of motion for the velocity.

6.2 Directions for Future Work

There are a number of possibilities for future research extending the work presented in this thesis.

Our use of the final winding statistics for the Kibble-Zurek mechanism investigation was in large part due to the inability to easily measure the number of solitons. Creating an effective procedure for this would provide a further test of the predictions of KZM and determination of critical exponents. Alternatively one could extend the investigation to a two or three dimensional Bose gas, where the topological defects are vortices. We already have a numerical framework for counting vortices, and the change in dimensionality may also lead to a different power law.

As there is yet to be agreement between experiments involving the Kibble-Zurek mechanism in Bose-Einstein condensation (e.g. [74, 80]), more experiments that test the critical exponents in detail need to be performed. Areas that may be fruitful include investigating the correlation length during quenches, to eliminate any affects from post-quench dynamics. This would also provide insight as to the true nature of the impulse regime, in particular the extent to which extent dynamics are truly frozen.

The relative values of the energy and number-damping rates were set such that the two processes were approximately equally weighted, however we do not know that this is necessarily the case. An investigation into the true values of these parameters, or just the relative value, would be useful for future applications of the stochastic projected Gross-Pitaevskii equation. Using the correct relative value of the damping rates may be crucial for finding the true critical exponents for the full SPGPE. The use of experimental parameters in determining these rates is also important for the modelling of experiments.

The analytical solutions of the soliton velocity equation of motion could provide a useful experimental technique for measuring the number of particle contained in bright solitons. Proposing an experiment to test these predictions and explore their usefulness in measurements is an obvious direction to take from these results.

The change of variables procedure we used for obtaining the bright soliton velocity stochastic differential equation was specifically for the energy-damping SPGPE. A more general procedure may be found for the full SPGPE. This could have important applications for systems where the spatially dependent wave function can be completely described by a small set of parameters, such as the dark soliton or a quantum vortex. Investigating these applications is an interesting future prospect.

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