

Bose-Einstein Condensation

Non-Equilibrium Studies of the Stochastic Gross-Pitaevskii Equation for Ultracold Atoms

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Abstract

Superfluids have fascinated the scientific community for nearly a century. Their unique properties were found to be caused by the phenomenon of Bose-Einstein condensation. We undertake a quantitative study of a zero temperature weakly-interacting atomic Bose gas through numerical simulation of the Gross-Pitaevskii equation. We introduce matter-wave dark solitons into an inhomogeneous atomic condensate and show that for multiple solitons their dynamics are modified by the exchange of sound energy. In this analysis we investigate an alternate interpretation to published work on the matter. We extend our study to finite temperature atomic Bose gases, which are best modelled by the stochastic Gross-Pitaevskii equation. This configuration unifies the condensate with low-lying thermal modes. At equilibrium, we established techniques from quantum optics to extract the condensate from the thermal cloud. We see how the introductions of spontaneous solitons are analogous to defects at the early Universe and how dissipation affects non-equilibrium excitations.

Contents

1	Introduction1.1A Brief History	3 3 4 6 6 9
2	Theoretical Framework 2.1 Derivation of the Gross-Pitaevskii Equation 2.2 Finite Temperature Theory 2.3 Numerical Analysis	10 10 14 18
3	Equilibrium Solutions to the 1D GPE3.1Uniform Solution3.2Wall Solution3.3Thomas-Fermi Approximation	20 20 20 21
4	Non-Equilibrium Dynamics of the GPE Solution4.1Opening the Trap4.2Dark Solitons	23 23 24
5	Stochastic GPE5.1The Finite Temperature Model5.2Equilibrium Analysis of SGPE5.3Non-Equilibrium Analysis of the DGPE5.4Non-Equilibrium Analysis of the SGPE	 29 31 35 36
6	Conclusions and Further Work	40
Α	Numerical Solution to a 1D Diffusion Equation	41
в	Origin of Wall Solution	43

Chapter 1

Introduction

1.1 A Brief History

The classical description of a particle is an object whose dynamics can be entirely described through its position and speed, which was the only description before 1905. However, post 1905 it was discovered that a particle's speed and position could not be a definite quantity, and was instead described probabilistically as a "quantum" particle. During this time a cloud of gaseous classical particles was well understood by describing the occupation of energy levels statistically, as defined by Ludwig Boltzmann. This approach was extended to include a description of a gas of quantum particles, which predicted the appearance of a *Bose-Einstein condensate*.

The road to Bose-Einstein condensation begins with a theoretical discovery made in 1924 by the Indian physicist Satyendra Bose [1] and Albert Einstein [2]. Bose sent Einstein a paper on the topic of quantum statistics, which impressed Einstein so much that he submitted it under Bose's name, and went on to write two more papers on the subject. The now coined Bose-Einstein condensate (BEC) is the result of their work.

A BEC is an unusual state of matter that can consist of millions of atoms, yet behave in synchrony as a single giant atom. In a BEC the weird phenomena of quantum mechanical systems, usually associated with the microscopic world, can be observed in the macroscopic domain, which gives us a completely new perspective of these once elusive properties. In this report we consider weakly-interacting, dilute (low density) atomic BECs. In order to create these systems, experimentalists needed to be able to engineer temperatures very close to absolute zero (zero Kelvin (0K) or -273° C), which was an obstacle for nearly 70 years. However, with advancements in cooling techniques through the 20th century the first BEC of this kind was experimentally observed in 1995 when, now Nobel prize winners Cornell and Wieman, succeeded in creating a condensate with rubidium-87 atoms (⁸⁷Rb [3], where 87 is the number of protons and neutrons in the nucleus of each atom) and Ketterle with sodium-23 atoms (^{23}Na) [4]. It is important to note that Bose-Einstein condensation is not limited to cold atoms, as we will see it comes about from a balance of density and temperature, such that if we increase both quantities a BEC can still be created. This means that they are also predicted to exist in neutron stars, where temperature is roughly 10^8 Kelvin [5]. As this discovery is so recent we are still in the process of uncovering new properties and uses of BECs. This state of matter is important in the field of physics because it has close analogies to many observable systems in nature, such as neutron stars, or even black holes, but importantly it is controllable in laboratory experiments.

The zero temperature dynamics of a BEC are accurately described by the Gross-Pitaevskii equation (GPE) [6, 7] as derived in the late 1950s, which is a classical fluid interpretation of the non-linear system. In the last 10 years much effort has also been put into describing more experimentally comparable predictions of finite temperature dynamics using stochastic methods. These introduce an element of random perturbation to our equation by considering fluctuations, e.g. such as those arising from particle interactions between the condensate and thermal particles.

1.2 Properties of Quantum Mechanical Systems

Here we present a brief overview of the important results from quantum mechanics that will be integral to our understanding of the BEC.

1.2.1 The Wavefunction and Phase

If we consider a particle described by classical mechanics we describe it by its position and momentum and predict its evolution using Newton's laws. The same cannot be said for quantum particles. Quantum mechanics tells us that particles are smeared out, or delocalised, over a region of space, referred to as small wavepackets. In order to describe this wave-like entity, we introduce the *wavefunction* $\psi(\mathbf{r}, t)$, which is in general a complex function that depends on time and position. For a single particle it defines the probability distribution, $P(\mathbf{r}, t)$, for finding the particle at position \mathbf{r} and time t according to

$$P(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2. \tag{1.1}$$

However, when we are considering multiple particles this describes the particle density, $n(\mathbf{r}, t)$, via

$$n(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2, \tag{1.2}$$

by integrating over all space we obtain the total particle number, N, i.e.

$$N = \int \mathrm{d}^3 \mathbf{r} |\psi(\mathbf{r}, t)|^2.$$
(1.3)

The wavefunction also holds properties relating to the systems phase. Phase is best explained with an example. Take a system of atoms with magnetic dipole moments, if the magnetic north of each atom is pointing in a random direction, the sum of the magnetic force across the whole system will be close to zero (as a particle with north facing down will cancel out with one facing up). In this system we call these particles *out of phase*. However, if we have a system with each moment facing the same direction, the sum will be strongly magnetic and the particles are *in phase*. When we cool a system down to a BEC the particles undergo a *phase transition* such that they are in phase, if we perturb one particle in this configuration all of the others react, hence they act collectively as one. It is this property of the BEC that gives it its close links to laser light. Lasers are a stream of photons that are all in phase. It is this similarity that gives a BEC the reputation of being an atom laser, or perhaps more jovially a "boser". We can define the phase by taking the definition of the density of particles from equation (1.2) and rearrange in terms of the wave function

$$\psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)}e^{i\theta(\mathbf{r},t)},\tag{1.4}$$

where θ is the phase of the system. We can rearrange this equation for θ by using Euler's formula for $\exp(i\theta)$ and separating the real and imaginary parts of the wavefunction to obtain

$$\theta(\mathbf{r}, t) = \arctan\left(\frac{\mathrm{Im}(\psi(\mathbf{r}, t))}{\mathrm{Re}(\psi(\mathbf{r}, t))}\right).$$
(1.5)

1.2.2 Pauli Exclusion Principle and Quantum Statistics

In nature, particles exist in two distinct categories, as defined by their "spin" (the particle's intrinsic angular momentum): bosons (particles with integer spin, e.g. light particles, called

photons) and fermions (particles with half-integer spin, e.g. electrons). Bosons are unbounded in their ability to occupy a single energy state. Fermions, however, are limited to only one particle per state by the *Pauli exclusion principle*, as discovered by Austrian physicist Wolfgang Pauli in 1925. Thus Bose-Einstein condensation ensues, as the name suggests, only for bosons, so that all of the particles can exist in the same state and behave as one. It is possible to take a pair of fermions (called a Cooper pair), whose spin will then be an integer, and create a condensate in a similar manner.



Figure 1.1: In each diagram the grey lines represent energy levels in a simple harmonic trap, a) shows a system of non-interacting bosons at T = 0 (red) in the lowest energy level and b) shows the same system with fermions (blue).

Statistics is used to describe large numbers of atoms, where it is not possible to track the position and momentum of each atom. We will quote the results used in quantum statistics [1, 2]. The number of bosons in an energy level ε_i is

$$N(\varepsilon_i) = \frac{g_i}{\exp\{(\varepsilon_i - \mu)/k_B T\} - 1} = \frac{g_i}{\exp\{\beta(\varepsilon_i - \mu)\} - 1},$$
(1.6)

where k_B is Boltzmann's constant, T is temperature, $\beta = 1/k_BT$, g_i is the degeneracy of state *i* (degeneracy is a measure of how prominent the quantum properties of the system are) and μ is the chemical potential, representing the energy required to add or remove particles from the system. The "-1" in the denominator arises from the fact that the particles are indistinguishable from one another. As $\varepsilon_i \to \mu$, $N(\varepsilon_i) \to \infty$, thus as we lower the energy of our system the number of particles in a lower energy level diverges. his means that bosons have the capacity to occupy the lowest energy level in vast numbers, the benchmark of Bose-Einstein condensation. This is in contrast to Fermi-Dirac statistics, where the number of fermions in an energy level ε_i is

$$N(\varepsilon_i) = \frac{g_i}{\exp\{\beta(\varepsilon_i - \mu)\} + 1},\tag{1.7}$$

where if we reduce the energy of a system such that $\varepsilon_i \to 0$ the number of Fermions in each state becomes $N(\varepsilon_i \to 0) = 1$, i.e. only one atom per state.

1.2.3 Commutators and Heisenberg's Uncertainty Principle

An operator is an object that acts on the state of the system to give a value, or even change the state, for example a derivative is an operator. Operators are often denoted with a "hat" above a symbol. For two operators \hat{A} and \hat{B} the *commutator* is defined as

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A},\tag{1.8}$$

which tells us whether the two values commute. If this quantity is zero for two observables \hat{A} and \hat{B} then we can measure them simultaneously, otherwise we are limited to how much information we can know about each of them at any instance in time. In quantum mechanics the *uncertainty principle* gives us a limit on how much information we can know about a system

at any given time. If we have two complimentary variables, for example in 1D a particle's position x and momentum p_x , then we have a lower bound on the precision to which we can truly know the values of each property simultaneously. Mathematically this is expressed by

$$\Delta p_x \Delta x \ge \frac{\hbar}{2},\tag{1.9}$$

where \hbar is the reduced Planck's constant and $\hbar \approx 1.055 \times 10^{-34}$ Js. Or correspondingly in operator notation, $[\hat{p}, \hat{x}] \neq 0$, i.e. the operators do not commute.

1.3 Superfluidity and Liquid Helium

Superfluidity is the name given to a system that exhibits a specific phase. This unique system is observed at extremely low temperatures, as required for weakly-interacting Bose-Einstein condensates and, as we will see, liquid helium. Superfluids have intrinsic properties that make them distinctive, such as no internal friction (viscosity). Due to this a superfluid has the ability to escape from an open top container, against the force of gravity, after applying some heat from underneath. This is commonly called the fountain effect. The road to the discovery of superfluid helium first started by the successful creation of liquefied helium in 1908 by Dutch physicist H. K. Ohnes, for which he earned the Nobel prize in 1914, with the phase transition occurring at around 4 Kelvin. A few decades later in 1937 Allen and Kapitza independently unveiled new properties of the fluid, the superfluid properties, by achieving temperatures at 2 Kelvin [8]. Fritz London [9] suggested using BECs to explain superfluidity, and under this assumption found the transition temperature of liquid Helium would be T = 3.13nK, which fits with the observed change in properties. So, to explain superfluidity we require a definition of Bose-Einstein condensation.

1.4 The Bose-Einstein Condensate

As shown in section 1.2.2, Bose-Einstein statistics tells us that the occupation of the ground state is unbounded as the energy of the system decreases. For dilute systems this can be achieved by reducing the temperature of a system below some critical T, given by T_c , such that the particles *want* to be in the lowest state. For a free gas of non-interacting particles in 3D, with particle mass m, this critical temperature is given by

$$T_{c} = \frac{2\pi\hbar^{2}}{mk_{B}} \left(\frac{n(\mathbf{r},t)}{\zeta(3/2)}\right)^{2/3},$$
(1.10)

where ζ is the Riemann zeta-function, defined as $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$, and $\zeta(3/2) \approx 2.612$. Below this temperature we would expect the onset of Bose-Einstein condensation. As mentioned at the beginning of the report a quantum particle is smeared out over a region of space as a wavepacket. When we decrease the temperature of a system, these wavepackets (whose typical size is given by the de Broglie wavelength) increase in length and begin to overlap, behaving as one giant matter wave. We can derive the thermal de Broglie wavelength by equating the quantum mechanical kinetic energy of free particles, $E_K = \pi k_B T$, with kinetic energy in terms of momentum, $E_{\rm kin} = p^2/2m$, and using the standard de Broglie wavelength $\lambda_{\rm dB} = 2\pi\hbar/p$ to obtain

$$\lambda_{\rm dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}},\tag{1.11}$$

where we note $\lambda_{\rm dB} \propto 1/\sqrt{T}$, so it increases in length as T decreases. Note that using equation (1.10) in terms of $\lambda_{\rm dB}$ we can write $n\lambda_{\rm dB}^3 \propto nT_c^{-3/2} \approx 2.612$. For Bose-Einstein condensation to occur this relation must be satisfied, and this is how systems such as neutron stars are expected to contain BECs because both density and temperature are much larger. The systems we are going to deal with are weakly-interacting dilute atomic Bose-Einstein condensates. Dilute refers to the low density, which means we require low temperatures. An important feature of dilute BECs, that we will use heavily in this paper, is that their zero temperature dynamics can be represented by a non-linear Schrödinger equation, which we derive in the next chapter. Figure 1.2 shows the BEC located in the lowest energy level of a simple harmonic trap.



Figure 1.2: A BEC confined in a bowl shaped simple harmonic trap. The BEC is found in the lowest energy level shown by the red line and the thermal cloud is the name given to the system of particles in the higher energy levels. The red line depicts the BEC density, where it is mainly found in the centre of the trap.

1.4.1 Experimental Realisation of BECs

Between prediction to experimental realisation of the atomic Bose-Einstein condensate there was a period of about 70 years. This is because in order to get cold atoms weakly-interacting we need low temperatures. For example, the temperature required for the rubidium experiment was $T_c \approx 100$ nK. So, how was this achieved back in 1995? We will discuss the cooling methods here, and how the images were taken that depict the phenomena. Typical atom numbers for a BEC experiment can vary between $N \sim (10^3 - 10^8)$, for example an experiment in 2007 with sodium atoms produced a BEC with atom number $N = 120 \times 10^6$ [10]. The information for this section was sourced from a talk given by one of the 1995 rubidium group's senior members, and Nobel prize winner, Eric Cornell [11].

Laser Cooling - $T < 1 \mu \text{K}$

All light carries a small momentum, when you stand outside on a sunny day there is a small force being applied to your body from the direction of the sun. This can be exploited by arranging this force so that it applies itself in all directions and keeps the individual atoms still, thus they will lose energy and cool. What we want is for an atom moving to the right to absorb a photon coming from the left in order to slow down. This is engineered using Doppler shift. Consider two lasers, one arrives at the north side of an atom and another south. Modulating the frequency of these lasers makes it possible to hold the atom still along this axis. By increasing the frequency (more "blue") slightly on one side, and decreasing the frequency on the other (more "red"), the atom is more likely to absorb the photon from the blue side and less likely to absorb the other from the red side. So, applying experimentally we use six lasers, two opposing lasers on each axis, and modulate the frequency accordingly. In the rubidium experiment this method cooled the system of bosons to be about $T \approx 300$ nK. The only thing that really stops this method from achieving lower temperatures is Brownian motion, which is where the atom absorbs a photon and spontaneously emits it in a random direction, giving rise to an observed jiggling motion.

Evaporative Cooling - $T \sim 100 \mathrm{nK}$

The next method begins by turning off the lasers that got us this far and instead using magnetic fields to hold the condensate in place in a bowl-like potential. In this configuration where the atoms with the most energy will be able to escape from the bowl, and those with the lowest energy sink into the bottom of the bowl. This is the premise of evaporative cooling. Cornell offers a simple analogy for this with coffee. When making a coffee there is often a lot of steam effervescing from the cup, atoms with high enough energy are leaving the surface of the liquid, evaporating away, leaving behind a coffee with a lower average energy. Thus, the coffee becomes colder after evaporation. Using this method only 2% of the density is lost after cooling by 20%. This is applied to the trapped BEC when the thermal atoms escape from the edges of the bowl-like trap, leaving colder atoms behind. We can effectively control the height of the bowl in time by using the properties of the atom to couple to controlled external radiation (in radiofrequency domain). Thus the trap is loosened slightly, removing higher energy atoms. What we are left with is a condensate of atoms at about $T \approx 100$ nK, as was the case for the rubidium experiment, but with a lower density than what was originally input into the system.

Imaging the Condensate

After creating the condensate we have to image it. These days it is possible to perform phasecontrast imaging [12], which lets us image the condensate without disturbing it. However, in 1995 a different method was used. In the rubidium experiment the atom number was too small to identify through conventional imaging techniques. To account for this the trap is turned off, letting the atoms fly apart. Then a laser light is shone onto the growing atomic cloud and the shadow created by the atoms is captured. This is called the expansion method of imaging. The condensate must first be destroyed before it can be imaged. This can lead to complications when wanting to experimentally verify non-equilibrium dynamics; any experiment will typically have to be destroyed and recreated multiple times to observe any time-dependent properties.



Figure 1.3: Images of the velocity distributions for the trapped atoms. On the left is the distribution for the thermal cloud, taken when the system is at a larger temperature than the critical temperature for BECs, the centre frame is a point in between that is part condensate and part thermal, and the final image is purely condensate within the density peak. The physical size of each image is 200μ m $\times 270\mu$ m and is taken after a period of about 0.04s. The colour represents density, with red as low density and white as high density and the lower the peak the more the atoms have moved since being released from the trap.

Figure 1.3 shows an image from the 1995 experiment depicting the velocity distribution; as

the time that the trap was released and the time of imaging is known, the velocity distribution is easily calculable. In this image the latitudinal axis (increasing to the right) in the rectangular image was under less confinement than the longitudinal axis. Observe how in the first image (left), where we just have a cloud of thermal atoms, the shape of the distribution is even in both planes (same radius from centre in all directions). However, in the final image (right), the condensate atoms are more "cylindrical" (larger radii along longitudinal lines) in shape. This is because in the thermal cloud we have the classical picture where the velocity distribution will be the same in each direction, irrespective of the confinement strength. The condensate is a quantum mechanical object, so Heisenberg's uncertainty principle takes hold. Heisenberg's says that the more you know a particle's position, the less you know its momentum, and vice versa. There is more confinement in the longitudinal axis, so we are more sure of the condensate's position and, as the object is more bunched up in coordinate space, it will spread out in momentum space. Hence, when we release the condensate from the trap it spreads out quicker in the confined axis, showing quantum mechanical behaviour in a macroscopic system.

1.5 Outline of Research

In this report we will discuss zero temperature models, for which an outline of the derivation is provided, describing weakly-interacting atomic BECs and we will present numerical models for a one-dimensional system. These were coded by the author in Fortran 95 and all subsequent figures from this output were created in MATLAB. Within this section of the report we derive analytic solutions through certain approximations and compare these to numerical equilibrium states. We then discuss time-dependent behaviour when we perturb the harmonic trap and consider the evolution of a system that contains macroscopic excitations of the Bose field called dark solitons. From this analysis we provide an alternate interpretation of an article published in Physical Review A.

We will also introduce finite temperature models, which arises from using theory from quantum optics to describe the differences between condensate and thermal particles. We need to introduce sophisticated techniques to extract the condensate contribution from the total density. In this section of the report the code used to generate the finite temperature realisations was kindly provided by the supervisor, Prof. Proukakis. The code is written in both Fortran 95 and C++ and has a complex web of multiple subroutines. All simulations were generated by the author, which required learning a new operating system, Unix, and learning how to apply this to the software Condor in order to run parallel jobs on up to 200 computers simultaneously. Using the numerical simulations we can reproduce similar perturbations to the zero temperature model, however whilst considering more realistic phenomena such as energy loss, collisions between the thermal and condensate particles, and particle fluctuations.

Chapter 2

Theoretical Framework

2.1 Derivation of the Gross-Pitaevskii Equation

Within the assumption of a dilute, weakly-interacting atomic Bose-Einstein condensate we can write down a *Hamiltonian* operator, \hat{H} , of a closed system with N atoms, which defines the total energy of the system. In the BEC we will only consider two contributions: single particle effects (\hat{h}_0 , where a particle might change state through interactions with the trap or random particle fluctuations) and from elastic binary collisions (\hat{V}_{int} , where "elastic binary" means we are assuming billiard ball like collisions and there is no energy loss from these collisions). Using these assumptions we can write down [13]

$$\hat{H} = \sum_{k=1}^{N} \hat{h}_0(\mathbf{r}_k) + \frac{1}{2} \sum_{k,l=1}^{N} \hat{V}_{\text{int}}(\mathbf{r}_k, \mathbf{r}_l), \qquad (2.1)$$

where the summations are over the positions of *every* particle in the system and the factor of 1/2 is necessary to prevent counting collisions between particles twice. From this we redefine the problem using what is known as the "occupation number representation" of second quantisation [14]. In this method we are no longer interested in the positions of the particles, but how many particles occupy each energy level and how they transition from level to level. There is a detailed discussion of this method in [13], from which we quote

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{h}_{0}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}^{\dagger}(\mathbf{r}') V_{\text{int}}(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}), \qquad (2.2)$$

where $\hat{\Psi}$ and $\hat{\Psi}^{\dagger}$ are the Bose field operators that destroy and create a particle, respectively, and describe the whole field including the condensate and thermal atoms. Generally $\hat{\Psi}(\mathbf{r},t) = \sum_i \psi_i(\mathbf{r}) \hat{a}_i(t)$, where ψ_i is the eigenstate wavefunction, \hat{a} and \hat{a}^{\dagger} are the operators that destroys and creates a particle, respectively [15]. $V_{\text{int}}(\mathbf{r} - \mathbf{r}')$ is the exact two-body interaction potential and $\hat{h}_0 = (\hbar^2/2m)\nabla^2 + V_{\text{ext}}$ is the single particle Hamiltonian, where m is the individual particle mass, V_{ext} is the potential energy, used to confine and control the system, and $(\hbar^2/2m)\nabla^2$ is the kinetic energy operator (compare to $E_{\text{kin}} = \hat{p}^2/2m$, with $\hat{p} = -i\hbar\nabla$). In equation (2.2) we read these terms from right to left, as they are operators. So the first term destroys a particle in one state $\hat{\Psi}$, acts upon that particle with the operator \hat{h}_0 , which may change the state the particle lies in, and recreates it in the new state with $\hat{\Psi}^{\dagger}$. Similarly for the second term we remove two particles from their initial states, they interact with some potential V_{int} , and they are then created in their new states.

We are working under the assumption of binary collisions, so our interaction potential can be expressed as $V_{\text{int}}(\mathbf{r} - \mathbf{r}') = g_{3D}\delta(\mathbf{r} - \mathbf{r}')$, where δ is the Dirac delta function, defined as $\int dx f(x)\delta(x - x_0) = f(x_0)$, and $g_{3D} = 4\pi\hbar^2 a_s/m$ is the coupling constant that defines the particle interactions. The constant a_s is the s-wave scattering length, which determines the size of the atomic interactions and is characterised by the atom used. We define a system as weakly-interacting if $a_s \ll \lambda_{\text{dB}}$. Substitution of the interaction potential into equation (2.2) then gives

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{h}_{0}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) + \frac{g_{3D}}{2} \int d\mathbf{r} \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}), \qquad (2.3)$$

where the dependence on \mathbf{r}' has been integrated out through the δ function. Now we state the Bose commutation relations

$$\left[\hat{\Psi}(\mathbf{r}'), \hat{\Psi}^{\dagger}(\mathbf{r})\right] = \delta(\mathbf{r} - \mathbf{r}'), \text{ and } \left[\hat{\Psi}(\mathbf{r}'), \hat{\Psi}(\mathbf{r})\right] = \left[\hat{\Psi}^{\dagger}(\mathbf{r}'), \hat{\Psi}^{\dagger}(\mathbf{r})\right] = 0, \qquad (2.4)$$

which also hold for $\mathbf{r} = \mathbf{r}'$. The first relation tells us that if one particle is created in one position and another destroyed in a different position, this cannot happen simultaneously. The second relation tells us that any two particles can be simultaneously destroyed or created, as long as they are *both* destroyed or *both* created.

Now we state and use the Heisenberg equation of motion to derive the system's dynamics, this equation describes a system where the state vector remains stationary and the operators evolve in time, giving

$$\begin{split} i\hbar\frac{\partial\hat{\Psi}(\mathbf{r}')}{\partial t} &= \left[\hat{\Psi}(\mathbf{r}'),\hat{H}\right],\\ &= \hat{\Psi}(\mathbf{r}')\hat{H} - \hat{H}\hat{\Psi}(\mathbf{r}'),\\ &= \hat{\Psi}(\mathbf{r}')\hat{H} - \int d\mathbf{r}\hat{\Psi}^{\dagger}(\mathbf{r})\hat{h}_{0}(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}')\\ &- \frac{g_{3D}}{2}\int d\mathbf{r}\hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}'),\\ &= \hat{\Psi}(\mathbf{r}')\hat{H} - \int d\mathbf{r}\left[\hat{\Psi}(\mathbf{r}')\hat{\Psi}^{\dagger}(\mathbf{r}) - \delta(\mathbf{r}'-\mathbf{r})\right]\hat{h}_{0}(\mathbf{r})\hat{\Psi}(\mathbf{r})\\ &- \frac{g_{3D}}{2}\int d\mathbf{r}\left[\hat{\Psi}(\mathbf{r}')\hat{\Psi}^{\dagger}(\mathbf{r}) - 2\delta(\mathbf{r}'-\mathbf{r})\right]\hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}),\\ &= \hat{\Psi}(\mathbf{r}')\hat{H} - \hat{\Psi}(\mathbf{r}')\hat{H} + \int d\mathbf{r}\hat{h}_{0}(\mathbf{r})\hat{\Psi}(\mathbf{r})\delta(\mathbf{r}'-\mathbf{r})\\ &+ g_{3D}\int d\mathbf{r}\hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r})\delta(\mathbf{r}'-\mathbf{r}). \end{split}$$

Here we have used the commutation relations to manipulate the order of the operators to move $\hat{\Psi}(\mathbf{r}')$. This then simplifies to

$$i\hbar \frac{\partial \hat{\Psi}(\mathbf{r}')}{\partial t} = \hat{h}_0(\mathbf{r}')\hat{\Psi}(\mathbf{r}') + g_{3\mathrm{D}}\hat{\Psi}^{\dagger}(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r}').$$
(2.5)

Now we have an equation that describes the motion of the whole field, however we want to extract information just on the condensate. We do this by splitting the Bose field operator into two parts [16]

$$\hat{\Psi}(\mathbf{r},t) = \hat{\psi}(\mathbf{r},t) + \hat{\delta}(\mathbf{r},t), \qquad (2.6)$$

which corresponds to an operator for the condensate part $(\hat{\psi})$ and the non-condensed, or thermal, atoms $(\hat{\delta})$. Under the approximation that there are a large number of atoms in the condensate the "hat" is dropped from the condensate operator and we are left with the condensate wavefunction ψ (and $\hat{\psi}^{\dagger} \rightarrow \psi^*$), which is a classical field approximation to the problem. This is because the operator acts on single particles, so when the particle number is large it will have no visible effect. If we substitute equation (2.6) into (2.3) we obtain

$$\hat{H} = H_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4, \qquad (2.7)$$

where,

$$H_0 = \int d\mathbf{r} \left[\psi^* \hat{h}_0 \psi + \frac{g_{3D}}{2} |\psi|^4 \right], \qquad (2.8)$$

$$\hat{H}_{1} = \int d\mathbf{r} \left[\hat{\delta}^{\dagger} \left(\hat{h}_{0} + g_{3\mathrm{D}} |\psi|^{2} \right) \psi + \psi^{*} \left(\hat{h}_{0} + g_{3\mathrm{D}} |\psi|^{2} \right) \hat{\delta} \right], \qquad (2.9)$$

$$\hat{H}_2 = \int d\mathbf{r} \left[\hat{\delta}^{\dagger} \left(\hat{h}_0 + 2g_{3\mathrm{D}} |\psi|^2 \right) \hat{\delta} + \frac{g}{2} \left((\psi^*)^2 \, \hat{\delta} \hat{\delta} + \psi^2 \hat{\delta}^{\dagger} \hat{\delta}^{\dagger} \right) \right], \qquad (2.10)$$

$$\hat{H}_{3} = g_{3\mathrm{D}} \int \mathrm{d}\mathbf{r} \left[\psi \hat{\delta}^{\dagger} \hat{\delta}^{\dagger} \hat{\delta} + \psi^{*} \hat{\delta}^{\dagger} \hat{\delta} \hat{\delta} \right], \qquad (2.11)$$

$$\hat{H}_4 = \frac{g_{3D}}{2} \int d\mathbf{r} \hat{\delta}^{\dagger} \hat{\delta}^{\dagger} \hat{\delta} \hat{\delta}.$$
(2.12)

Each term is categorised by the number of $\hat{\delta}$ terms it contains. If we take an ideal system, i.e. no interactions, in the limit of zero temperature we find that all of the particles are in the condensate so our non-condensate operator $\hat{\delta}$ can be ignored. This is a valid approximation for $T \ll T_c$ and when the system is weakly-interacting. Thus if we take the Heisenberg motion equation (2.5) and substitute $\hat{\Psi} = \psi$ we obtain the Gross-Pitaevskii equation (GPE) [6, 7]

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + g_{3\text{D}}|\psi(\mathbf{r},t)|^2\right)\psi(\mathbf{r},t).$$
(2.13)

Here the energy density for any point in space is given by equation (2.8), thus the total energy of the BEC in this approximation is given by

$$E = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r}, t)|^2 + V_{\text{ext}}(\mathbf{r}) |\psi(\mathbf{r}, t)|^2 + \frac{g_{3\text{D}}}{2} |\psi(\mathbf{r}, t)|^4 \right].$$
(2.14)

The GPE conserves both particle number, N, and energy, E. Note that if $g_{3D} < 0$ the interactions between particles are *attractive* as it reduces energy to put particles together, if $g_{3D} > 0$ the interactions are *repulsive* as it costs energy to put particles together and if $g_{3D} = 0$ there are no interactions. This equation with $g_{3D} = 0$ is simply called the Schrödinger equation, which models the dynamics of a single particle. It is also a good approximation to a multiple, interacting, particle system of bosons because bosons act as a single entity and can be considered as one large particle.

We will be analysing equilibrium properties of the system. We can extract static solutions by making the substitution $\psi(\mathbf{r}, t) = \psi_0(\mathbf{r})e^{-i\mu t/\hbar}$, where $\psi_0(\mathbf{r})$ is the time-independent system eigenstate and μ is the chemical potential, as appearing in the Bose-Einstein distribution function. Inserting this into equation (2.13) we obtain the *time-independent GPE*

$$\mu\psi_0(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + g_{3\text{D}}|\psi_0(\mathbf{r})|^2\right)\psi_0(\mathbf{r}).$$
(2.15)

We note that this equation is identically satisfied when the Hamiltonian of this equation is equal to μ . Thus, as the energy of the system approaches the chemical potential we obtain equilibrium solutions. Using this result the equation that we will take forward is a slightly modified GPE, given by

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + g_{3\text{D}}|\psi(\mathbf{r},t)|^2 - \mu\right)\psi(\mathbf{r},t).$$
(2.16)

In this model we have used several assumptions: for our interaction parameter we assume that collisions between only *two* atoms have occurred, which realistically depends on the density of

the fluid. We also assumed that collisions do not alter the systems energy (elastic collisions). The error involved with making these assumptions however is decreased by the nature of the system we are looking at. For a system of lower density, collisions will be infrequent and affect our approximation less. In a dilute BEC the density is of the order $(10^{13} - 10^{15})$ cm⁻³, comparable to air at room temperature of the order 10^{22} cm⁻³ [17].

In this report we will consider the evolution of a 1D system. In this case (2.16) becomes [18]

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi(x,t)|^2 - \mu\right)\psi(x,t) = \hat{H}_{GP}\psi(x,t), \qquad (2.17)$$

and we define $\hat{H}_{GP} = -\hbar^2 (\partial^2 / \partial x^2) / 2m + V(x) + g |\psi(x,t)|^2 - \mu$. We have now introduced g as the one dimensional interaction constant, which is scaled as $g = g_{3D}/2\pi l_{\perp}^2$, where $l_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$ and ω_{\perp} are the harmonic oscillator width and trapping frequency in the y and z directions, respectively.

2.1.1 Potential

We will consider two cases for the form of the potential: a uniform background potential $V_{\text{ext}}(\mathbf{r}) = 0$, in which the Bose-Einstein condensate is not constrained in any space and will spread out, and the case with a simple harmonic trap by setting the potential to be $V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m \left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right]$, where ω_j is the angular trapping frequency in the *j* direction (sometimes called the quantum harmonic oscillator frequency). To model the homogeneous zero potential in 1D we consider a box of finite length, such that the walls of the box have infinite potential. This confines the system within the walls, such that in between there is zero potential. In a non-interacting case we solve Schrödinger's equation to find that the n^{th} energy level is $E_n = (\hbar^2 \pi^2/2mL^2) n^2$, for a box of length *L*. The ground state energy for this system comes from substituting n = 1 into the energy relation. Note that $E_1 > 0$. This is a powerful result, because it tells us that even at zero temperature there will still be some energy. Figure 2.1 shows this schematically.



Figure 2.1: The energy is shown for the first three states, with the equivalent wavefunction solutions. These are given by $\psi_n = \sqrt{2/L} \sin(k_n x) \exp\{-i\omega_x t\}$, with wavenumber $k_n = n\pi/L$.

For the 3D simple harmonic oscillator, in a non-interacting system, the discrete energy for the n^{th} level can be shown to be $E_{jn} = \hbar \omega_j (n + 1/2)$. Again, the lowest energy possible still has some energy with $E_{j0} = \hbar \omega_j / 2$ (for n = 0). For both of these potentials in an interacting system the energy relation is to all intents and purposes similar, but the levels are closer together for low n.

We are working in 1D, so we need to reduce this into trapping solely in the x direction. Consider the case where $\omega_y = \omega_z = \omega_{\perp}$ and $\omega_x \ll \omega_{\perp}$. This produces the situation in the figure



Figure 2.2: A simple harmonic trap, in the interacting case, with the trap frequency in the x direction set to be much lower than y and z, i.e. $\omega_x \ll \omega_{\perp}$. Each green line represents a energy level and the red line is the energy of the system E.

2.2. Here we see that the energy levels in the traps defined by ω_{\perp} are bound by the energy relation $E \approx \hbar \omega_{\perp} (n + 1/2) \gg \hbar \omega_x (n + 1/2)$ and thus each level is further apart. In the figure we have placed a red line across some energy level E. If the energy of the system is at this level much of the condensate will settle in the lower levels in the x direction and on the lowest possible level in the y and z traps. If we were to try and force the system into the next energy level in ω_{\perp} we would require a high influx of energy, so we are confining the condensate into changes in the x-direction only. Thus, we can model a simple harmonic trap in 1D by setting $V(x) = \frac{1}{2}m\omega_x^2 x^2$, if we take $\omega_x \ll \omega_{\perp}$, such that the transversely it remains in the harmonic oscillator (Gaussian) ground state.

2.1.2 Dimensionless Gross-Pitaevskii Equation

Many of the parameters in the GPE are cumbersome to work with numerically, for example $\hbar \sim 10^{-34}$ Js, and for rubidium $m \sim 10^{-25}$ kg and $g \sim 10^{-39}$ Jm. We note that $\hbar \omega_x$ has units of energy, Joules, and we define the harmonic oscillator ground state width $l_x = \sqrt{\hbar/m\omega_x}$ as a length scale. Using these we can transform

$$\begin{split} \mu \to \tilde{\mu} &= \frac{\mu}{\hbar\omega_x}, \ x \to \tilde{x} = \frac{x}{l_x}, \ g \to \tilde{g} = \frac{g}{\hbar\omega_x l_x}, \\ \psi \to \tilde{\psi} &= \sqrt{l_x} \psi \ \text{and} \ t \to \tilde{t} = \omega_x t. \end{split}$$

We can substitute these into equation (2.17), with a simple harmonic trap potential, to give

$$i\frac{\partial\tilde{\psi}}{\partial\tilde{t}} = \left(-\frac{1}{2}\frac{\partial^2}{\partial\tilde{x}^2} + \frac{1}{2}\tilde{x}^2 + \tilde{g}|\tilde{\psi}|^2 - \tilde{\mu}\right)\tilde{\psi}.$$
(2.18)

We can also derive a similar equation for a uniformly zero potential, which is identical but without the $\tilde{x}^2/2$ term. We will use this equation when solving numerically, as it is more convenient. The values we obtain from this analysis will then be rescaled so that they have physical meaning and can be compared to experimental observations.

2.2 Finite Temperature Theory

In this section we will outline some of the theory required for finite temperature models. At T > 0 there are particles that exist in both condensate and thermal states, which means that when estimating the density of the condensate we have to take certain measures to make sure we separate the two. With the thermal excitations there is an element of random noise that will be different each time the experiment, or numerical simulation, is run. To account for this numerically we run as many simulations as possible and average over them by taking the "ensemble average". This will show us the most common outcome and reduces the effect of

random perturbation. There is a link between energy dissipation and these random perturbations called fluctuation-dissipation theory. This means that fluctuations drive the strength of the noise and vice versa.

2.2.1 Quantum Correlation Functions

Correlation functions are used in quantum optics to define a system's coherence, where a perfectly coherent system is one that has equal phase throughout, such as a laser. Penrose and Onsager [19] gave the precise definition of a Bose-Einstein condensate as

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \langle \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}(\mathbf{r}') \rangle \to \text{constant}, \qquad (2.19)$$

between two positions \mathbf{r} and $\mathbf{r'}$. This means the condensate is coherent through off-diagonal long-range order (ODRLO, i.e. in the limit $|\mathbf{r} - \mathbf{r'}| \to \infty$). To acquire the true density from by the Penrose-Onsager definition one must numerically diagonalise the matrix to find the largest eigenvalue; this eigenvalue will correspond to the macroscopically populated state, the BEC.

The correlation functions were derived to help distinguish between coherent laser light and normal light. For the BEC, they highlight the differences between condensate and thermal atoms. In classical systems, particles are coherent up to a length scale of $\lambda_{\rm dB}$, whereas for a pure homogeneous BEC in an infinite system we would expect the coherence length to tend to infinity, i.e. when we perturb one particle in the system all of the other particles should react. The, normalised, first-order correlation function is a measure of coherence length, and is defined as [20]

$$g^{(1)}(\mathbf{r},\mathbf{r}') = \frac{\langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r}')\rangle}{\sqrt{\langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})\rangle\langle \hat{\Psi}^{\dagger}(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\rangle}},$$
(2.20)

where $\langle \dots \rangle$ represents the ensemble average over simulations. When we are just considering the condensate wavefunction this is

$$g^{(1)}(\mathbf{r},\mathbf{r}') = \frac{\langle \psi^*(\mathbf{r})\psi(\mathbf{r}')\rangle}{\sqrt{\langle |\psi(\mathbf{r})|^2\rangle\langle |\psi(\mathbf{r}')|^2\rangle}} = \frac{\langle \psi^*(\mathbf{r})\psi(\mathbf{r}')\rangle}{\sqrt{\langle n(\mathbf{r})^2\rangle\langle n(\mathbf{r}')^2\rangle}}.$$
(2.21)

This is measured between two particles at positions \mathbf{r} and \mathbf{r}' , where we are measuring at equal time, so there is no time dependence. When analysing this function we plot the value of $g^{(1)}$ against the distance between the two particles, $|\mathbf{r} - \mathbf{r}'|$. If $g^{(1)} = 1$ then we have perfect coherence between the two particles, $g^{(1)}$ then tends to zero when their separation is greater than their coherence length. If the Bose gas has undergone condensation this value should to tend to a constant as $|\mathbf{r} - \mathbf{r}'| \to \infty$, which defines the appearance of a condensate through ODLRO, as described above.

Now we introduce the second-order coherence function. In quantum optics, this is used to determine the correlation of two separate photon-detection events and highlights the difference between a classical and quantum-mechanical system [21]. It is used in BECs to provide a contrast to a system that could be either described by the classical mechanics of matter waves from a thermal source or those that have the theoretical properties associated with the quantum field of a BEC. So, the second-order coherence function is defined as [20]

$$g^{(2)}(\mathbf{r},\mathbf{r}') = \frac{\langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}^{\dagger}(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})\rangle}{\langle \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})\rangle\langle \hat{\Psi}^{\dagger}(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\rangle}.$$
(2.22)

Generally this is evaluated at zero separation $(\mathbf{r} = \mathbf{r}')$. So, for the condensate wavefunction only this reads

$$g^{(2)}(\mathbf{r},\mathbf{r}) = \frac{\langle |\psi(\mathbf{r})|^4 \rangle}{\langle |\psi(\mathbf{r})|^2 \rangle^2} = \frac{\langle n(\mathbf{r})^4 \rangle}{\langle n(\mathbf{r})^2 \rangle^2}.$$
(2.23)

This result takes on the value $g^{(2)} = 2$ for normal light (thermal particles), and $g^{(2)} = 1$ for laser light (condensate particles).

2.2.2 Onset of Bose-Einstein Condensation in One and Three Dimensions

Equation (1.10) is the temperature at which the onset of Bose-Einstein Condensation begins in 3D for an ideal gas in a trap, and corresponds to the point at which phase and density fluctuations are suppressed. Lower temperatures mean a higher proportion of the atoms will become in phase. Consider figure 2.3, where we have compared the proportion of atoms in the ground state, N_0/N against temperature for both 1D and 3D systems [22]. In the left graph



Figure 2.3: a) Schematic for the 3D case. As the temperature drops below T_c the atoms, N, begin populating the ground state, N_0 , until they are equal at T = 0. b) In 1D we always find some particles in the ground state, but the rate at which they are affected by temperature is different.

(a) we find the gradient to steepen as the temperature decreases below T_c , this highlights the aforementioned point that the particles want to be in the ground state. However in our 1D system, b), we find a linear relationship, so this phenomena is suppressed. In our 1D system we do not have the same critical temperature given by $T = T_c$, instead we have three temperatures of note for an ideal 1D gas. Firstly, Ketterle and van Druten [23] considered non-interacting particles found within a harmonic potential. They found that macroscopic occupation of the ground state occurs at

$$T_{QC} = \frac{\hbar\omega_x}{k_B} \frac{N}{\log(2N)},\tag{2.24}$$

which is only valid for large, but finite, N. The subscript QC stands for quasi-condensate, which signifies a state in which pockets of condensate are in phase, but not all pockets are identical. The behaviour of this state is much like the BEC, however it does not have longrange order. In the interacting case there are two temperatures that characterise 1D quantum degenerate gases [24]. The degeneracy temperature is

$$T_d = \frac{N\hbar\omega_x}{k_B},\tag{2.25}$$

and below this temperature density fluctuations are suppressed. The third temperature is defined to reduce fluctuations in the phase and density, as given by

$$T_{\phi} = \frac{N(\hbar\omega_x)^2}{\mu k_B} = \frac{\hbar\omega_x}{\mu} T_d \ll T_d.$$
(2.26)

Note that $T_d > T_{QC} > T_{\phi}$. The effects these temperatures create will be important when discussing finite temperature models. We can analyse these effects by comparing the first order correlation functions for each of them. In figure 2.4 we look at the effects of dimensionality for



Figure 2.4: a) Schematic for a 3D first order correlation function for two particles, at \mathbf{r} and $\mathbf{r'}$, confined in a trap of length *L*. *b*) A 1D schematic. See [25] for more details.

 $g^{(1)}$ on the coherence length $(L_{\rm coh})$. We find that in a 3D system thermal particles are coherent only when they overlap, i.e. the distance between them is less than the deBroglie wavelength, and that when $T \ll T_c$ we see the onset of Bose-Einstein condensation across the length of our system. The value of the constant $g^{(1)}$ plateaus to is determined by the proportion of density in the lowest energy level. This can be expressed as $n_{\rm BEC}/n_{\rm tot}$, where $n_{\rm BEC}$ is the density of the Bose-Einstein condensate and $n_{\rm tot}$ is the total density of the system. In 1D, the temperature region $T_{\phi} < T < T_{QC}$ produces a quasi-condensate, where the coherence length is longer than the deBroglie wavelength but does not stretch to the entire length of the system. We see that any coherence length greater than the red diagonal line, given by $T \simeq T_{\phi}$, is considered to be a good approximation to a "true" BEC, with lower temperatures giving larger portions of the density in $n_{\rm BEC}$. In both cases $g^{(1)}$ never becomes completely constant because of the limited size of the system, only if $L \to \infty$ can we observe ODLRO.

2.2.3 Approximate Condensate Extraction

When considering finite temperature models we note that some of the density profile, n(x), we generate will be thermal particles, and the rest will be the BEC, which we are interested in extracting. We observe the quasi-condensate when the temperature is reduced below the threshold T_{QC} . In this range density fluctuations are suppressed, such that pockets of the solution are in phase and considered as Bose condensed, but the system as a whole is not completely in phase. We can use the second order correlation function to extract the proportion of the condensed density, that falls within these conditions, by taking [26]

$$n_{\rm QC}(x) = n_{\rm tot}(x)\sqrt{2 - g^{(2)}(x, x)},$$
 (2.27)

because for thermal particles $g^{(2)} = 2$ and condensed particles $g^{(2)} = 1$. Now we have a model for the quasi-condensate, but for a full model we must find an approximation suppressing phase fluctuations too. These phase fluctuations are defined by the first coherence function, $g^{(1)}$. So we can define [27]

$$n_{\text{BEC}}(x) = \lim_{|x| \to \infty} n_{\text{tot}}(x) g^{(1)}(0, x) \sqrt{2 - g^{(2)}(x, x)}.$$
(2.28)

This method suppresses both density and phase fluctuations and leaves us with just the BEC. However, this is just an approximation as it is defined for large distances only. For short range analysis this method loses information. This is because the first order correlation function must give $g^{(1)}(0,0) = 1$, as well as the minimum coherence length being the deBroglie wavelength, so density near the centre is generally over-estimated at all temperatures.

2.3 Numerical Analysis

2.3.1 Imaginary Time Propagation

We introduce a handy trick which we will use for numerically solving the Gross-Pitaevskii equation. Consider the wavefunction as a superposition of eigenstates, where $\psi_m(x)$ is an eigenstate of the wavefunction $\Psi(x,t)$, and expressed as in terms of eigenenergies E_m . We write

$$\Psi(x,t) = \sum_{m} \psi_m(x) e^{-iE_m t/\hbar},$$
(2.29)

where it is important to note that each next eigenstate has higher energy than the previous one, or $E_m > E_{m-1}$. Now make the substitution $t \to -it$, then we have

$$\Psi(x, -it) = \sum_{m} \psi_m(x) e^{-E_m t/\hbar}.$$
(2.30)

Crucially, the eigenenergy governs the decay rate, and so the eigenstate with the lowest energy (the ground state of the system) decays slowest. This can be easily seen by taking $\exp(-E_0t/\hbar)$ out as a factor of equation (2.30), then

$$\Psi(x, -it) = e^{-E_0 t/\hbar} \left(\psi_0 + \psi_1 e^{-(E_1 - E_0)t/\hbar} + \psi_2 e^{-(E_2 - E_0)t/\hbar} + \dots \right),$$
(2.31)

and here it is clear that the terms with greater exponents will decay quicker as t increases. Thus by taking an approximation of the initial profile of the wavefunction during propagation in imaginary time the thermal states will dissipate, leaving behind the ground state. However, as the factor of $\exp(-E_0 t/\hbar)$ is also tending towards zero as $t \to \infty$ we have to limit the number of simulations in imaginary time before we lose the condensate as well.

2.3.2 The Crank-Nicolson Method

We introduce the notion of *finite differences* by considering the familiar first derivative

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$
(2.32)

In this case, the finite difference is the expression f(x+h) - f(x), when we divide by h we get the difference quotient. We could similarly use f(x+h/2) - f(x-h/2), which is easier to use when defining the second derivative. When evaluating the derivative numerically we will not be able to reduce the value of h to zero, however we will obtain more accurate solutions for a smaller step size. For second order differentiation we obtain

$$f''(x) = \lim_{h \to 0} \frac{f'(x+h/2) - f'(x-h/2)}{h} = \lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$
 (2.33)

The Crank-Nicolson method uses finite differences to numerically solve partial differential differential equations. It was developed by John Crank and Phyllis Nicolson in the 1950s [28]. For a partial differential equation, in one dimension, it can be said

$$\frac{\partial u}{\partial t} = F\left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}\right).$$
(2.34)

Letting $u(j\Delta x, n\Delta t) = u_j^n$ the Crank-Nicolson method is the calculation of

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{1}{2} \left[F_j^{n+1} \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right) + F_j^n \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right) \right].$$
(2.35)

Note that the numerical calculation of a second order derivative defined in equation (2.33) is now given by

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} + \mathcal{O}(\Delta x^2).$$
(2.36)

In many cases the algebraic problem is a tridiagonal matrix, which is zero everywhere except in the main diagonal and the diagonals above and below (often reffered to as sup- and subdiagonals). These matrices can be solved with the tridiagonal matrix, or Thomas, algorithm [28] (see appendix A for example). From this reference we note that the method only converges if the relation $\Delta t/(\Delta x)^2 < 1/2$ holds. Consider equation (2.18) in the form $i\partial \psi(x,t)/\partial t = \hat{H}_{GP}\psi(x,t)$, for the Hamiltonian \hat{H}_{GP} . Direct integration gives

$$\psi(x, t + \Delta t) = \exp\{-i\Delta t \hat{H}_{GP}\}\psi(x, t) + \mathcal{O}(\Delta t^2), \qquad (2.37)$$

assuming the Hamiltonian is fixed during the time interval. We can replace the exponential function using a finite difference approximation called Cayley's form [29]

$$\exp\{-i\Delta t(H-\mu)\} = \frac{1 - \frac{i\Delta t}{2}\hat{H}_{GP}}{1 + \frac{i\Delta t}{2}\hat{H}_{GP}} + \mathcal{O}(\Delta t^2).$$
(2.38)

We now have the tools to evolve our solution in time and space. On letting $\psi(j\Delta x, n\Delta t) = \psi_j^n$ the full time evolution step is

$$-\frac{i\Delta t}{4(\Delta x)^2}\psi_{j-1}^{n+1} - \frac{i\Delta t}{4(\Delta x)^2}\psi_{j+1}^{n+1} + \left[1 - \frac{i\Delta t}{2}\left(\mu - \frac{1}{(\Delta x)^2} - V_{\text{ext}}(x) - g|\psi_j^{n+1}|^2\right)\right]\psi_j^{n+1}$$
$$= \frac{i\Delta t}{4(\Delta x)^2}\psi_{j-1}^n + \frac{i\Delta t}{4(\Delta x)^2}\psi_{j+1}^n + \left[1 + \frac{i\Delta t}{2}\left(\mu - \frac{1}{(\Delta x)^2} - V_{\text{ext}}(x) - g|\psi_j^n|^2\right)\right]\psi_j^n, \quad (2.39)$$

which can be written as a tridiagonal matrix and solved using a simple algorithm. However, in the left hand side of this equation we have a non-linear term that depends on the value of ψ^{n+1} . We can get around this by letting $\psi^{n+1} = \psi^n$ for one iteration and substituting the newly obtained ψ^{n+1} back into the original equation. This intermediate process is repeated until convergence of the new wavefunction, although we find that one iteration gives sufficient accuracy.

Chapter 3

Equilibrium Solutions to the 1D GPE

We have introduced all of the necessary notation and methods to numerically solve the 1D, dimensionless, GPE at zero temperature. Everything we consider in this chapter will be a condensate, as we are not accounting for the thermal particles. When solving numerically we will use some typical experimental parameters to try and obtain realistic results. An example recent experiment with rubidium atoms had a system of N = 1700, with trapping frequencies $(\omega_x, \omega_\perp) = (53 \text{ Hz}, 890 \text{ Hz})$. The mass and scattering length of rubidium is $m = 1.44 \times 10^{-25} \text{kg}$ and $a_s = 5.05 \times 10^{-9} \text{m}$, respectively. We will use $(\omega_x, \omega_\perp) = (2\pi \times 20 \text{ Hz}, 2\pi \times 500 \text{ Hz})$, which using our equation for the interaction strength corresponds to $g = 0.1046\hbar\omega_x l_x$. The particle number depends on our choice of the chemical potential and trapping frequency, we derive a formula for this quantity later in the chapter.

3.1 Uniform Solution

Firstly we will look at the analytical solution for a problem where we have a uniform potential, defined by taking $V_{\text{ext}}(x) = 0$. In this form there is no trap confining the BEC. As such the background potential is homogeneous, i.e. there are no spatial variations, thus any derivatives in x are zero. In this case equation (2.15) becomes $\mu \psi = g |\psi|^2 \psi$, which has solution $\psi(x) = \psi_{\infty} = \sqrt{\mu/g}$, or, in terms of the density

$$n(x) = n_{\infty} = |\psi_{\infty}|^2 = \mu/g.$$
 (3.1)

Thus the BEC wavefunction and density are constant in space in an infinite-sized $V_{\text{ext}}(x) = 0$ system. We will use this result when plotting solutions to the wavefunction, as we know that gn(x) should have a value of μ away from any potential confinement, thus we have an immediate check for our solution.

3.2 Wall Solution

The uniform solution will only match up with experiments far away from a barrier either side of the condensate. However, to have something reasonable to compare with experiments we must analyse that happens within a confined BEC. Consider an infinite hard wall placed at x = 0, with potential defined by $V_{\text{ext}}(x) = 0$, for x > 0 and $V_{\text{ext}}(x) = \infty$, for $x \leq 0$. We note that no particles can exist outside of the range $x \leq 0$, as to pass through the barrier would require infinite energy. This gives the boundary condition $\psi(0) = 0$. Meanwhile away from the wall the potential energy is zero, so ψ will return to its bulk wavefunction giving the second condition $\psi(x \to \infty) = \psi_{\infty} = \sqrt{\mu/g}$. We are currently considering static properties, so our $\partial/\partial t$ term is zero, however for $x \geq 0$ the wavefunction obeys

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + g|\psi|^2\psi = \mu\psi.$$
(3.2)

We prove the solution to this equation in appendix B, however we just state it here to be

$$\psi(x) = \psi_{\infty} \tanh\left(\frac{x}{\xi_h}\right),$$
(3.3)

where we define ξ_h as the *healing length* and $\xi_h = \hbar/\sqrt{mgn_{\infty}}$, or in dimensionless units (on noting ξ_h is a length) $\tilde{\xi}_h = 1/\tilde{\mu}$. The healing length is defined as the thickness of the layer from zero density at the wall to the equilibrium value, due to particle interactions with the barrier wall.

Now we will consider the numerical simulation for this problem. Let us consider a wall placed at x = 0 and take the dimensionless chemical potential to be $\tilde{\mu} = 30$, which means physically we have $\mu = 30\hbar\omega_x$ and $V_{\text{ext}} = 0$ for the wall solution at x > 0. We know, using equations (3.1) and (3.3), the dimensionless analytical solution to the right of the barrier is

$$\tilde{\psi}(\tilde{x}) = \sqrt{1500} \tanh\left(\sqrt{30}\tilde{x}\right). \tag{3.4}$$

Figure 3.1 a) shows the analytical and numerical results, with one overlaying the other. Here we only see little discrepancy between the two, giving us confidence with the accuracy of our numerical results. For our parameters the healing length is $\xi_h \approx 0.2l_x$, which we have marked on the figure as a red dotted line. So, it is at this point that particle-wall interactions stop having an effect and we return to the n_{∞} solution. This solution can also be redefined for a



Figure 3.1: a) The numerically obtained wall solution in (solid) black with the analytical solution overlaid in (dashed) blue are in good agreement. We have marked the point of the healing length from the wall as a dotted red line. b) The density (red) for the an infinite potential well with $\tilde{g} = 0.1046 > 0$, with same solution for g = 0 (blue).

square well of width $L \gg \xi_h$, i.e. a barrier placed at x = 0 and x = L. As long as the well is wide enough the wavefunction tends to zero at both edges with the same tanh-like behaviour, and tends to n_{∞} in the centre. Figure 3.1 b), shows the infinite box solution both with and without interactions. Note how we obtain the ground state solution as shown in figure 2.1 for the non-interacting case. When g > 0 the interactions broaden and flatten the density profile since they introduce an energetic cost to having a high density of atoms in one place, however if there are no interactions the particles will be more inclined to move to the centre.

3.3 Thomas-Fermi Approximation

In this section we use the form of the potential as described in section (2.1.1) as a harmonic trap. Now we consider the interactions to be strongly repulsive. Under this assumption the effect of the kinetic energy, $\nabla^2 \psi$ -term, is negligible in comparison. This is known as the *Thomas-Fermi approximation*. The time-independent GPE then simplifies to $\mu \psi = g |\psi|^2 \psi + V_{\text{ext}} \psi$. Rearranging for the density $n(x) = |\psi|^2$ and inserting $V_{\text{ext}}(x) = \frac{1}{2}m\omega_x^2 x^2$ gives

$$n(x) = \frac{2\mu - m\omega_x^2 x^2}{2g}.$$
 (3.5)

We note that as $|x| \to \infty$ the density will become negative, which is non-physical, so we truncate this beyond the n(x) = 0 boundary. This boundary is called the *Thomas-Fermi* radius, and, from substitution of $x = R_{\rm TF}$ into equation (3.5), satisfies $\mu = m\omega_x^2 R_{\rm TF}^2/2$. The corrected Thomas-Fermi density profile (with $R_{\rm TF}$ being substituted in) is then

$$n(x) = \frac{m\omega_x^2 \left(R_{\rm TF}^2 - x^2\right)}{2g} \Theta(R_{\rm TF}^2 - x^2), \qquad (3.6)$$

where $\Theta(x)$ is the *Heaviside* function, defined as $\Theta(x) = 0$ for x < 0 and $\Theta(x) = 1$ otherwise. This gives us an inverted parabola with the greatest density at the centre. When we substitute x = 0 we obtain $gn(x) = \mu$, so the maximum density should be equal to the chemical potential. We can use this relation for the density to find the number of atoms within the Thomas-Fermi profile

$$N = \int_{x} n(x) dx = \int_{-R_{\rm TF}}^{R_{\rm TF}} \frac{m\omega_x^2 (R_{\rm TF}^2 - x^2)}{2g} dx = \frac{4m}{6g} R_{\rm TF}^3 \omega_x^2.$$
(3.7)

Then substituting in the relation for R_{TF} we can solve this in terms of μ to give

$$N = \frac{2}{3} \frac{(2\mu)^{3/2}}{q\omega_x \sqrt{m}}.$$
(3.8)

Substituting the parameter transformations from the dimension analysis we find this simplifies to $N = 2^{5/2} \tilde{\mu}^{3/2}/3\tilde{g}$. When considering problems in a simple harmonic oscillator we should now know how many atoms we expect to find in our condensate, given our experimental parameters. If we choose $\mu = 30\hbar\omega_x$ we can use equation (3.8) to find that we are modelling a system with $N \approx 3000$ particles. Next, we show the numerical realisation of the dimensionless equation for a simple harmonic oscillator with the same parameters as previous, this gives equation (3.6) to be $n(\tilde{x}) = 25(60 - \tilde{x}^2)\Theta(60 - \tilde{x}^2)$. Figure 3.2 shows this simulation, with the analytical results and the harmonic trap potential overlaid. We note the slight difference at the Thomas-Fermi



Figure 3.2: *a*) Numerical density (black solid line) with the Thomas-Fermi profile (green dot-dashed line) overlaid. The harmonic trap is also shown (red solid line) with a separate axis (red). *b*) The size of the discrepancy at the Thomas-Fermi radius, which we find is equal to the healing length ξ_h . *c*) The phase (blue solid line) of the system.

radius, i.e. at $x = \pm \sqrt{60} l_x$, highlighted in figure 3.2 b). These discrepancies are given by the healing length, ξ_h , where particle interactions give enough thermal energy to move slightly further out of the trap than the Thomas-Fermi limit allows. These simulations are useful in our discussion of the equilibrium states of BECs, however the important factor is whether we are observing a thermal cloud or a Bose-Einstein condensate; this is why we plotted the phase of the system. We see from figure 3.2 c) that there is a strong indication that we are observing a system with a BEC as the particles have undergone a phase transition and, within the Thomas-Fermi radius, are completely in phase.

Chapter 4

Non-Equilibrium Dynamics of the GPE Solution

Any non-equilibrium analysis where we make a sudden change to the energy is called a *quench*. Here we will perform a variety of quenches that have all been experimentally achieved in the last twenty years and serve as a good test of the Gross-Pitaevskii theory. We use the same parameters as the previous chapter for consistency.

4.1 Opening the Trap

In this section we will instantaneously change the trap frequency: $\omega_x \to 0.9\omega_x$, which in experimental terms means reducing the frequency of the laser confining the BEC. Numerically we account for this by taking $V_{\text{ext}}(\tilde{x}) = \tilde{x}^2/2 \to V_{\text{ext}}(\tilde{x}) = 0.9^2 \tilde{x}^2/2$. The trap potential is parabolic, by reducing the frequency we are essentially "widening" the trap, creating less of a hold on the condensate. This quench will be performed after running in imaginary time and obtaining the equilibrium ground state solution. Figure 4.2 shows how the trap potential changes. Consider how this scenario would work classically if we had fluid contained in a bowl,



Figure 4.1: The original trap for the simple harmonic oscillator (black dotted line) and the trap after the frequency has been modulated (blue solid line). The change in frequency creates a wider trap and forces the discrete energy levels to be lowered and forced closer together.

in a somewhat rounded shape such as the harmonic oscillator. If the bowl is suddenly widened then we would expect to see the fluid fill the gaps created around the rim, and to see the fluid oscillate briefly between the newly defined rim and the centre, until internal viscosity causes the system to come to a halt. In figure 4.2 we see what happens to the density of the BEC after this quench. Plot a) is a *carpet* plot, which shows the density profile changing over time, with red as high density and blue as low. The profile "breathes" in and out with each oscillation. From equation (3.8) we note that $N \equiv N(\mu, \omega_x)$. Thus, if we change the trap frequency we should also change the particle number. However, this value does not change because in the



Figure 4.2: *a*) A carpet plot that follows the density over time. For $t < \omega_x^{-1}$ we ran in imaginary time to reach the equilibrium solution then we propagate in real time after applying the quench. We see periodic peaks and troughs where the density profile becomes broad and flat, then returns to the thinner density with a higher peak. *b*) This plot shows how the central density, n(0), oscillates in height over time.

GPE particle number is conserved. Instead all that we have done is reduce the confinement on the BEC and reduce the value of the lowest energy level ($E_0 \approx \hbar \omega_x$). The BEC wants to relax at the lowest density, as shown in b), but as there is no energy or particle loss it is forced to oscillate indefinitely. When the central density is at a trough in b) we see a wider profile in a), due to the constant number of atoms.

4.2 Dark Solitons

A dark soliton is a local decrease in wave amplitude and has the following properties: they move along the density profile without changing shape, they are localised within a region and two solitons can interact with each other and come out of the collision unchanged, except for a slight phase shift [30]. In a classical fluid this non-linear wave would dissipate through viscous damping, but in a superfluid or BEC there is no viscosity, so these disturbances remain.

4.2.1 Experimental Creation of Dark Solitons

Atomic dark solitons have been achieved experimentally by either perturbing the atomic density [31] or by phase imprinting [32, 33]. Phase imprinting is where a laser beam illuminates a small portion of the condensate such that that portion acquires a phase shift, but it is not left on long enough to perturb the density as a whole. Dark solitons are also expected to appear after the collision of two condensates [34, 35]. In 3D solitons have been observed to exist up to lifetimes of the order 10ms, however in 1D systems they are expected to remain in the condensate to the order of several seconds [36].

4.2.2 Dark Soliton Solution

We can simulate the instantaneous introduction of a soliton into the system by multiplying the steady condensate solution, as produced at the end of the imaginary time propagation, by the solution for a soliton. The wavefunction will then maintain its shape but have a sharp decline in density at a point $x = x_0$ and as we propagate through time this point will oscillate along the profile. A dark soliton is described by the wavefunction [32]

$$\psi_{\rm ds}(x,u,t) = \sqrt{n_{\infty}} \exp\left\{-i\frac{\mu t}{\hbar}\right\} \left(\sqrt{1-u^2} \tanh\left[\frac{x-x_0}{\xi_h}\sqrt{1-u^2}\right] + iu\right),\tag{4.1}$$

where: n_{∞} is the homogeneous background density, as described in section (3.1); u = v/c, v represents the velocity of the soliton, $c = \sqrt{n_{\infty}g/m}$ is the Bogoliubov speed of sound in the medium and u is contained in the range $0 \le u \le 1$ (i.e. $0 \le v \le c$); and x_0 represents the initial central position of the soliton. The soliton will always be implemented at t = 0, so the exponential term can be neglected and we will write $\psi_{ds}(x, u, 0) \equiv \psi_{ds}(x, u)$. It is important to note that if u = 0 then the soliton created is called a *black* soliton and has zero density in the BEC, but maximum soliton energy (conversely a u = 1 soliton has zero soliton energy). This type of soliton cuts the density profile in half and due to its non-dispersive nature has been compared to a particle with negative mass. In fact, for weak forces to a first order, this categorisation has been shown to hold [37] and it is this idea that a tells us that the dark soliton will oscillate back and forth under harmonic confinement. As we have effective negative mass the momentum of the soliton is given by $p = -m_{ds}u$. Thus from the balancing of the forces from Newton's second law (F = ma) and the harmonic oscillator restoring force (F = -kx, for some positive constant k) to first order, we can state the harmonic equation of motion as [38]

$$\frac{d^2 x_{\rm ds}}{dt^2} = -\frac{\omega_x^2}{2} x_{\rm ds},$$
(4.2)

which has oscillatory solutions with frequency $\omega_{\rm ds} = \omega_x/\sqrt{2}$, and thus period $\tau_{\rm ds} = 2\pi\sqrt{2}/\omega_x$.

The solution for ψ_{ds} produces a soliton in a uniform potential, but works as a good estimate for dark solitons in a simple harmonic trap. Figure 4.3 shows a range of velocities of dark



Figure 4.3: a) Dark solitons in a uniform background density, in separate runs, with $\psi_{ds}(x, u = 0)$ (black solid), $\psi_{ds}(x, u = 0.25)$ (blue dotted), $\psi_{ds}(x, u = 0.5)$ (green dot dashed) and $\psi_{ds}(x, u = 0.75)$ (red dashed). b) The phase profile for each dark soliton.

solitons created in a $V_{\text{ext}}(x) = 0$ background potential. There is a relationship between the depression density (n_d) , change in phase (S referred to as the phase slip) and soliton speed (u), expressed as $u = \sqrt{1 - (n_d/n)} = \cos(S/2)$. Hence a phase slip $S = \pi$ gives u = 0 and corresponds to a black soliton. Smaller phase slips correspond to solitons that are not as deep but propagate at greater speeds. If we were to leave the solution to propagate in real time in figure 4.3 a) each soliton would oscillate back and forth through the medium, as opposed to dissipating or remaining stationary.

4.2.3 One Soliton Solution

Now we can use this to model a dark soliton in a simple harmonic trap. Figure 4.4 shows a dark soliton with dimensionless speed u = 0.4 inserted into the equilibrium solution at real time t = 0 then left to oscillate in the BEC. We see that the dimensionless period is given by $\tau_{\rm ds}/\omega_x = \tilde{\tau}_{\rm ds} = 2\pi\sqrt{2} \approx 8.89$. The dark soliton propagates to the right with dimensionless speed u = 0.4 until the central point of the soliton has zero density at some point $x = x_{\rm c}$, where $x_{\rm c}$ is a critical x value. Then it cannot move any further to the right so changes direction until

it reaches the opposite critical value of $x = -x_c$ on the left. This process repeats and the dark soliton is seen to be oscillating with period $\tilde{\tau}_{ds}$. After the soliton oscillates freely for a while there is a small build up of density on top (hence the maximum density is $gn(x) \approx 31\hbar\omega_x$ in d)), this is energy being transferred as sound waves. It is important to note there is no energy loss in these systems, any energy given up by the soliton as sound is often reabsorbed later from the background medium. In figure 4.5 we plot the same time evolution as figure 4.4, but



Figure 4.4: A dark soliton created in the Thomas-Fermi profile with $\psi_{\rm ds}(x, u = 0.4)$. We follow the solution in time from its inception (t = 0), to the point where it hits zero density and begins to oscillate back towards the centre $(t = 2.2\omega_x^{-1})$, the same point on the other side $(t = 6.7\omega_x^{-1})$ and back to the centre for one full oscillation $(t = 8.9\omega_x^{-1})$.

showing the phase of the system at each snapshot. As the phase is calculated through an arctan function the possible values are restricted between the range $(-\pi/2, \pi/2)$. As such, plots b) and c) show phase slips for black solitons, as the density is zero at these points, hence why there is a sudden π phase shift in each of these plots. We note that initially there is a clean phase slip across the centre of the profile. However after propagating in time, outside of the Thomas-Fermi radius is very noisy. This is because the solution ψ_{ds} is clean for a homogeneous background and picks up noise when applied to the harmonic trap.



Figure 4.5: Evolution of the phase of the dark soliton, at the same times and positions shown in figure 4.4.

We can also demonstrate that the oscillation period is the same, irrespective of the value

u in $\psi_{\rm ds}$. Figure 4.6 shows the central position of a dark soliton for three different values of u. Here we see that the change in soliton depth is proportional to the change in soliton speed, given by the gradient of the trajectory, thus giving each soliton a different amplitude but the same period of oscillation. From this figure it can also be confirmed that the period is $\tilde{\tau}_{\rm ds} \approx 8.89$.



Figure 4.6: The oscillatory motion of the dark soliton, observed with $\psi_{ds}(x, u = 0.2)$ in blue (solid), $\psi_{ds}(x, u = 0.4)$ in green (dashed) and $\psi_{ds}(x, u = 0.6)$ in red (dotted).

4.2.4 Sound Mediated Dark Soliton

In this section we model the case where two solitons are inserted simultaneously into the condensate. We look at a paper published by Allen *et al.* [39], where the authors consider one black soliton in the centre of the density profile and another dark soliton placed off-centre. We have used the same parameters as the paper to try and recreate the results as much as possible. Figure 4.7 shows the nature of this solution as a carpet plot. If we follow the dark soliton,



Figure 4.7: The density, indicated by colour, changing over time with the introduction of two solitons, one near black ($x_0 = 0, u = 0.1$) and one dark ($x_0 = -3l_x, u = 0.3$). We have used the variables $\mu = 30\hbar\omega_x$ and $g = 0.1046\hbar\omega_x l_x$.

which is the soliton with a wide amplitude when introduced, we see that it gains energy, thus it slows down and its amplitude decreases. The system we are modelling has constant energy, so if one soliton is gaining some energy the other must be losing the same amount. This is exactly what happens as the black soliton we started with, u = 0.1, has near maximum energy and gives some of it up to begin oscillating with a wider amplitude. This energy transfer is due to sound waves. Unlike the single soliton case, the sound is not reabsorbed by the same soliton but is absorbed by the soliton with lower energy.

The explanation given in Allen *et al.* says that this energy transfer continues until the solitons become comparable in energy and then the process reverses. In this interpretation the soliton that is initially black (has the lowest amplitude) bounces off of the dark soliton at the point of equal energy. However, on looking at the simulations in figure 4.7 the author of this report believes that this interpretation is incorrect. Instead, the solitons do not bounce off each other, but instead they pass through each other; as described by Drazin and Johnson [30]. In this scenario the energy transfer continues until the soliton that starts with the least energy, gains the maximum amount of energy allowed by the system. When it has obtained maximum energy this process starts to reverse (in figure 4.7 this first occurs at $t \approx 150\omega_x^{-1}$). We can analyse this accuracy of this interpretation by considering the period of the solitons. The correct interpretation will have a roughly constant period (roughly due to soliton collisions), as derived for the single soliton case.



Figure 4.8: The period of oscillation for each soliton. The black solid line shows the period for the soliton that is initially black and the blue dashed line shows the period for the soliton that is initially dark. We extended the simulation to $t = 300\omega_x$ for a broader analysis. *a*) The Allen *et al.* interpretation of results. *b*) The author's approach.

So, in figure 4.8 we have plotted the period of oscillation over time for each soliton. From the Allen *et al.* interpretation the period has a large and unexpected increase, with a corresponding decrease, in each soliton repeated every $t \approx 100\omega_x^{-1}$. This gives strong evidence for our interpretation of the results. These jumps do not occur in our interpretation, so are explained if the solitons pass through each other. However, we also find a sharp increase in the length of the period at several times (i.e. $t \approx 125\omega_x^{-1}$) in both interpretations. When referring back to the carpet plot these times correspond to one soliton with maximum, and the other minimum, energy. For two optical solitons in a system, it has been shown that soliton period scales inversely with amplitude [40], i.e. $\tau_1/\tau_2 \sim A_2/A_1$, for amplitudes A_1 and A_2 . Thus as the black soliton has the shorter amplitude $(A_1 < A_2)$ it will also have the longest period $(\tau_1 > \tau_2)$, which is exactly what we observe in figure 4.8. A further investigation is required to fully understand the meaning of the results. For example, we could look at the speed of each soliton to determine why these changes in period are sometimes sudden and other times exhibit gradual change.

Chapter 5

Stochastic GPE

5.1 The Finite Temperature Model

In this chapter we analyse finite temperature systems. We can model this by considering the following approximate split: we define the system (ϕ) as the condensate and low-lying thermal cloud (found below an appropriate cut-off energy level), and the heat bath, which contains purely thermal particles. This is shown schematically in figure 5.1. Again, in this formulation we are not interested in the individual positions of each particle, rather the number of atoms at each energy level.



Figure 5.1: We have split up our field into two parts, beneath the cut-off point (E_{cut} , thick black line) is taken to be the BEC and the low thermal particles, and above the cut-off energy level is a purely thermal part. We have also shown a particle transfer/collision, which we will describe as each particle being annihilated from their initial states and created in their new states.

Consider the following analogy: imagine going to the river Tyne with a kettle of boiling water. After pouring the kettle water into the river the water will reach a very quick thermal equilibrium with no overall change to the river's temperature. This analogy is similar to our set up here, we have a system of a much lower temperature to its surroundings that will have no effect on the heat bath's dynamics other than particle transfer at the edge of our cut-off point. Hence we take the heat bath to be steady. We are now trying to solve the system defined by a Langevin equation called the stochastic Gross-Pitaevskii equation (SGPE) [41]

$$i\hbar \frac{\partial \phi(x,t)}{\partial t} = \hat{H}_{GP}\phi(x,t) - iR(x,t)\phi(x,t) + \eta(x,t), \qquad (5.1)$$

where -iR is the *dissipation* of atoms from the system (represented by the transfer of atoms between the system and bath; mathematically it is calculated assuming the instant destruction of a particle in one state and creation of a particle in another state) and η represents *fluctuations* in the system, which is an additive stochastic term. This means every individual run will be different because we are adding a random number to each time-step. We then take the average over runs to analyse the data.

5.1.1 Fluctuation and Dissipation

The dissipation can be calculated by setting [41]

$$-iR = \frac{1}{2}\hbar\Sigma^{k}(x) \left[1 + 2N(\varepsilon)\right]^{-1},$$
(5.2)

where Σ^k , which is a fluctuation term (called the Keldysh self energy), and $N(\varepsilon)$ is the Bose-Einstein distribution from section (1.2.2). We can expand this to first order as

$$-iR \simeq \frac{\beta}{4}\hbar\Sigma^k(\varepsilon - \mu),$$
 (5.3)

where $\beta(\varepsilon - \mu) \ll 1$ and $(\varepsilon - \mu)$ is comparable to the Hamiltonian \hat{H}_{GP} . We can write our stochastic GPE as

$$i\hbar\frac{\partial\phi}{\partial t} = (1 - i\gamma)\hat{H}_{GP}\phi + \eta, \qquad (5.4)$$

where $-i\gamma = \beta \hbar \Sigma^k/4$. This parameter is an approximation for the dissipation of our system. When simulating data we will take a constant value of γ to be

$$\gamma = \frac{12ma_s^2 k_B T}{\pi \hbar^2},\tag{5.5}$$

as derived in [42]. We note that $\gamma \propto a_s^2 T$ and $\gamma \sim 10^{-2}$ for the considered temperature range. This also governs the rate that our solution reaches equilibrium, which will be slower for lower temperatures. We take this small constant to be our initial condition for ϕ , because in an experiment we would start with no condensate atoms and the BEC density will grow with time, which is what we will see later. However, when we are looking at equilibrium dynamics we can speed up this growth process by multiplying γ by a factor of 10, say. The rate at which the solution reaches equilibrium under this regime will be entirely non-physical, but the final steady state solution shall be the same, which we have checked to be the case. Equation (5.4) without noise is the dissipative Gross-Pitaevskii equation (DGPE), which describes the dynamics of the condensate in the presence of a steady thermal cloud. The solution of the DGPE is the average outcome of the SGPE.

The Gaussian noise has correlations in the Langevin field equations given by [41]

$$\langle \eta^*(x,t)\eta(x',t')\rangle = 2\hbar\gamma k_B T\delta(x-x')\delta(t-t').$$
(5.6)

This relation represents the fluctuation-dissipation theorem for the system, as it describes the magnitude of the relationship between the fluctuation strength and damping parameter, γ . In general, a stochastic ODE is of the form

$$dx(t) = -\Omega x(t)dt + \sigma dw(t), \qquad (5.7)$$

where w(t) is a random noise and Ω is a constant. We can calculate a solution from an initial time t_0 to be

$$x(t) = e^{-\Omega(t-t_0)}x(t_0) + \sigma e^{-\Omega t} \int_{t_0}^t e^{\Omega t'} \mathrm{d}w(t').$$
(5.8)

To apply this method to the SGPE we must first write equation (5.4) as

$$d\phi(x,t) = -\frac{i}{\hbar} \left[\alpha \hat{H}_{GP} \phi(x,t) dt + \eta(x,t) dt \right], \qquad (5.9)$$

where $\alpha = 1 - i\gamma$. Then to solve this we use the approach described by Bijlsma and Stoof [43], but first discussed in [44], to solve for a time increment from t_j to $t_j + \Delta t$. They derived the time step

$$\phi(x_j, t_j + \Delta t) = \exp\left[-i\alpha \hat{H}_{GP} \Delta t/\hbar\right] \left\{\phi(x_j, t_j) - \xi(x_j, t_j)\right\},\tag{5.10}$$

where

$$\xi(x_j, t_j + \Delta t) = \frac{i}{\hbar} \exp\left[-i\alpha \hat{H}_{GP} \Delta t/\hbar\right] \int_{t_j}^{t_j + \Delta t} dt' \exp\left[-i\alpha \hat{H}_{GP} \Delta t/\hbar\right] \eta(x_j, t').$$
(5.11)

Here ξ is the redefined fluctuation term whose correlations now take the form

$$\langle \xi_m^*(x,t)\xi_n(x',t')\rangle = 2\hbar\gamma k_B T\delta(x-x')\delta_{mn}\Delta t + \mathcal{O}(\Delta t^2), \qquad (5.12)$$

where δ_{mn} is the Kronecker delta, defined as $\delta_{mn} = 1$ if m = n or $\delta_{mn} = 0$ otherwise. Following [45] the classical field $\xi \propto \sqrt{i\Sigma^k} \sqrt{\Delta t/\Delta x}$ when simulating numerically, so smaller spatial discretisation creates larger noise. We see from equation (5.10) that to implement the noise we subtract the random number from ϕ at each time step.

5.1.2 Choosing the Energy Cut-off Point

The energy cut-off point, $E_{\rm cut}$, between the low thermal and purely thermal energy levels is defined as

$$E_{\rm cut} = \frac{2\pi}{(\Delta x)^2}.\tag{5.13}$$

So, in this approximation the amount of low thermal levels we include depends on our discretisation. Smaller Δx gives more particles in our simulation, and the more noise we simulate through ξ . This means we have to keep Δx low enough so that we don't include too much of the thermal cloud, but high enough so we satisfy the convergence properties of the Crank-Nicolson method (highlighted in section 2.3.2).

5.1.3 Condor High Throughput System

To simulate the data we used a program called Condor, which makes use of idle processors on the University campus to calculate many parallel jobs. Once a program is ready to go it is sent to the Condor collector, which then distributes jobs to machines as soon as they are available. If someone logs onto a computer that is currently being used by Condor the job breaks. It is then sent back to the collector and resubmitted to a new processor, continuing the simulation from the breaking point with no loss of data. This system also uses a seed to make sure the random variable is consistent after being restarted. Once the data is collected it is averaged over runs to infer the mean behaviour of the gas. Without access to Condor this last chapter would not have been possible. To give an idea of how much of a difference access to this package has made, one simulation from the SGPE at a low temperature could take 20 minutes. To get a smooth average we typically run 1000 simulations. If each run was being made one after another this would take just under 2 weeks to simulate. However, with Condor we generally have access to at least 200 processors at any given time, so this takes less than 2 hours.

5.2 Equilibrium Analysis of SGPE

In this section we will begin to analyse data from the SGPE code. Note that the analytical GPE solutions from chapter 3 are still the benchmark for comparison, as they contain information of the pure BEC. The first experiment that required stochastic analysis was done in 1998 with sodium-23 atoms (²³Na) [46]. So, in this chapter we will use the parameters for sodium, which are an atomic scattering length $a_s = 2.75$ nm and mass $m = 3.818 \times 10^{-23}$ kg. We will also

use the trapping frequencies $(\omega_x, \omega_{\perp}) = (2\pi \times 150 \text{ Hz}, 2\pi \times 400 \text{ Hz})$, unless stated otherwise, which makes $g = 0.0364\hbar\omega_x l_x$. However, we are now considering the effect of temperature as well, which is dependent on μ . The atom number also is temperature dependent, so in the SGPE we will only use equation (3.8) as an approximation to the true value. Using the formula for T_{ϕ} in equation (2.26) with $\mu = 30\hbar\omega_x$ we calculate that $T_{\phi} = 275$ nK. Often when considering temperature analysis it is useful to make comparisons to T/T_{ϕ} , as if $T/T_{\phi} < 1$ we are considering systems in the region where both phase and density fluctuations are suppressed.

Before analysing the effect of each variable in the SGPE, we will show a simple equilibrium solution. Figure 5.2 shows a single run against its averaged counterpart, over 200 simulations.



Figure 5.2: a) A single, noisy, simulation from the SGPE (black) and an ensemble average over runs (red). b) A few snapshots taken from the numerics as the density grows in time. Parameters chosen were $\mu = 35\hbar\omega_x$ and T = 100 nK ($T/T_{\phi} = 0.33$, for chosen μ), corresponding to a system of N = 1400 sodium atoms.

We see that the shape of the density profile is much like the expected zero temperature equivalent, however as we will see, part of this density is condensate, part thermal cloud. Figure 5.2 b) shows the increase in density in time, with the particle number equilibrating at $t \approx 200 \omega_x^{-1}$.

Now we are considering finite temperature models the main difficulty is in distinguishing between the condensate and the thermal particles. We have already mentioned much of the theoretical framework required to extract the condensate in chapter 2, so here we will implement these models.

5.2.1 Effect of Temperature

To analyse the temperature dependence we will plot three averaged results from the SGPE with T = 100 nK $(T/T_{\phi} = 0.3)$, $T = T_{\phi}$ and T = 600 nK $(T/T_{\phi} = 1.89)$. We will use $\mu = 40\hbar\omega_x$, which corresponds to a system with N = 1760. The density plots, shown in figure 5.3 *a*), are remarkably similar. This emphasises the point that it is difficult to immediately see which one of these has the largest proportion of condensed atoms. We can see that for higher temperatures the central density is lower, and the density profile is wider. This is because there are more thermal particles for larger T. The thermal particles are forced to the edges of the trap, due to repulsive interactions, and thus create a larger density in the region $|x| > R_{TF} \approx 7.7 l_x$.

We have also plotted the first order correlation function, figure 5.3 b), that shows the coherence length, $(L_{\rm coh})$, from the centre of the trap outwards, where we have just plotted for positive x. We see that for T_{ϕ} the condensate is coherent up to the Thomas-Fermi radius, as expected from section 2.2.1. We also see that for $T < T_{\phi}$ we have a strong coherence up to about $x = 6l_x$, where the value dips because of the finite size of the system. Similarly, for $T > T_{\phi}$ we see that the coherence length is much shorter than the Thomas-Fermi radius, and is within the quasi-condensate range because $T_{QC}/T_{\phi} = 4.9$.

The second order correlation function for the various temperatures in shown in figure 5.3 c). We note that for a true BEC this should be precisely 1 within the Thomas-Fermi radius and



Figure 5.3: a) The density profile for three different temperatures, as shown as proportions of T_{ϕ} . b) The first order correlation function for these three realisations of the SGPE. c) The corresponding second order correlation function, where we have also overlaid the value for a pure BEC (red dashed line) within the Thomas-Fermi radius.

2 within the thermal cloud. What we observe is similar for the lower temperatures, however as we increase the temperature we see more thermal particles, and greater noise, within the Thomas-Fermi range as well.

Within a finite system it is difficult to tell what the true coherence length is for the condensed particles. For every temperature shown, $g^{(1)}$ is forced to tend to zero as the solution approaches the Thomas-Fermi radius. We can, however, use the behaviour before the coherence length is affected by the boundary to extrapolate an approximation to the "true" coherence length in an infinite system. The shape of the curve changes from a Gaussian relationship to an exponential one with increasing temperature, implying the change from a true condensate to a quasi-condensate [47]. From figure 5.3 b) we can see that $g^{(1)}$ has an exponential slope for temperatures $T \gg T_{\phi}$ and a Gaussian for $T \ll T_{\phi}$, so when fitting the curves we will use the function f(x), which contains information on both types. f(x) is defined by [27]

$$f(x) = e^{-\left[x/L_{\rm coh} + \alpha(x/L_{\rm coh})^2\right]},$$
(5.14)

where $L_{\rm coh}$ is the coherence length and α is a parameter that defines how much control the Gaussian profile has over the estimation. We expect large α for Bose condensed particles and small α for thermal particles. We applied this fit to the range of temperatures shown above



Figure 5.4: a) The coherence length obtained by fitting the data to a Gaussian-exponential fit to predict the behaviour at infinity. b) The linear relationship between the central point of the second order correlation function and temperature, or $g^{(2)}(0,0) \propto T$.

and included two extra points for T = 10nK $(T/T_{\phi} = 0.03)$ and T = 900nK $(T/T_{\phi} = 2.83)$ to obtain a slightly wider range of effects. Figure 5.4 *a*) shows the results for the values of $L_{\rm coh}$ against temperature. We note that for temperatures greater than T_{ϕ} we have low coherence lengths. However, as $T_{QC}/T_{\phi} = 4.9$ all of the data shown is in the quasi-condensate range, so much of the cloud is condensed in separate pockets of matter. Each of these pockets has a different phase, hence the lack of coherence through the system as a whole. For temperatures less than T_{ϕ} we see these regions of quasi-condensate become in phase and there is a steep increase in the coherence length. Another interesting by-product of this analysis is the linear relationship between the central value of $g^{(2)}$ and temperature, shown in figure 5.4 b). We find that the number of thermal particles entering the central region is directly proportional to T, which can be derived analytically to be [48]

$$g^{(2)}(0,0) = 1 + \frac{4\sqrt{2}}{3} \left(\frac{T}{T_d}\right).$$
(5.15)

5.2.2 Approximate Penrose-Onsager Solution

From the last discussion we have seen how the temperature affects the correlation functions. If we return to the formulae as presented in section 2.2.3 we saw that these functions extract the condensate from the thermal cloud. As mentioned, this approximation is valid for particle separations tending to infinity. So, using this we show the approximate Penrose-Onsager profile for the case T = 100 nK in figure 5.5. From this figure we see that the profile maintains mostly



Figure 5.5: Approximate Penrose-Onsager solution for $T/T_{\phi} = 0.3$ (blue) and the thermal particles from the same data (red). This stresses the point made earlier that the thermal particles are pushed to the sides of the density profile. The low thermal cloud solution was calculated by taking the total density (black dashed) and subtracting the approximate Penrose-Onsager density, leaving only particles outside of the ground state.

the same shape, except has a "spike" at the top, which is non-physical. This is because the approximation always multiplies the central density by $g^{(1)}(0,0) = 1$, when really there will be some thermal particles included in that region. Currently we are forcing the number of thermal particles in the centre to be near zero, which as shown in figure 5.4 b) is only true for T = 0. Despite this, the approximation itself is very accurate, and becomes more so for larger x. Hence we can conclude that we have extracted the Bose-condensed atoms from the thermal cloud to a high degree of accuracy.

5.2.3 Effect of Varying Δx

In this section we are going to compare some numerical results with those found in a paper published by Bijlsma and Stoof [43]. In this paper they used the SGPE in the way we have described in this chapter, however the figure in question is testing the numerics to make sure they match for a non-interacting thermal cloud and assessing the effects of changing the parameter Δx for fixed Δt . To create a non-interacting thermal cloud we need to set g = 0 and $\mu < 0$ as these correspond to no interactions and to thermal particles, respectively. From figure



Figure 5.6: A steady density profile of a non-interacting gas, above the critical temperature T_c . Here we used $\Delta t = 0.002 \omega_x^{-1}$ and the discretisation Δx varied from the green line: $\Delta x = 0.05 l_x$, blue line: $\Delta x = 0.2 l_x$ and the red line: $\Delta x = 0.8 l_x$. As the problem we are simulating is entirely classical we have overlaid the exact solution expected. The chemical potential used was $\mu = -5\hbar\omega_x$, the temperature was set to T = 400 nK. The one-dimensional trapping frequency was set to $\omega_x = 2\pi \times 13$ Hz and $\omega_{\perp} = 2\pi \times 500$ Hz. We modelled this system based on Sodium atoms (²³Na), with an atomic scattering length $a_s \approx 2.75$ nm and $m = 3.818 \times 10^{-23}$ kg. Compare with [43], where they have used more averaging to get smoother results.

5.6 we see that if we decrease the value of Δx the density profile grows, this is because we are including higher energy levels and thus more thermal particles. We also see an increase in the noise, even after averaging over one thousand simulations, due to the relation for ξ . It can be shown that the density distribution for thermal particles is a Gaussian curve, however the slope in figure 5.6 can be described by a Lorentzian curve. This is a limitation of the SGPE due to the classical approximation for the field ξ . This Lorentzian curve appears for the higher temperatures in figure 5.3 *a*), describing the growing thermal cloud. In figure 5.3 *a*) we could find a Gaussian fit over the condensate particles (between the Thomas-Fermi radius) and use the relation for the thermal contribution, shown in [43], to provide a fit for $|x| > R_{\rm TF}$.

5.3 Non-Equilibrium Analysis of the DGPE

For this analysis the code was written by the author, as we do not require Condor for a single observation. We already have a GPE model, so to extend into the DGPE multiply the Hamiltonian by the factor $(1 - i\gamma)$ and set $\gamma = 0.01$.

5.3.1 Solitons in the DGPE

In the previous chapter we obtained a non-equilibrium solution for a dark soliton. If we now progress in the same fashion with a damped system we can follow the soliton's progress through the density, as demonstrated in figure 5.7. We see that the period of oscillation remains constant, which is what we would expect as the size of the soliton does not affect this value. However, the amplitude of the soliton increases as the soliton loses energy, until the soliton is damped out at around $t \approx 30\omega_x^{-1}$. From figures 5.7 b) and c) we can see that the jump in phase reduces at later times, corresponding to a lower energy soliton.



Figure 5.7: *a*) Following the central position of the soliton (the point with the lowest density) as it oscillates through the BEC. *b*) The initial phase profile when the soliton is introduced and moving right. *c*) The phase of the system at $t = 18.5\omega_x^{-1}$, when the soliton is moving left.

5.3.2 Opening the Trap in the DGPE

Consider the GPE solution where we quenched the trapping potential, in section 4.1. In a real system we would expect some energy loss after time has passed, whereas figure 4.2 shows the solution returning to the maximum density after each oscillation. If we use the DGPE for a system of rubidium atoms, with the same parameters as section 4.1, we can simulate this dissipation by taking $\gamma = 0.01$. We display the central density against time in figure 5.8. Here we see that the system loses energy and slowly tends to a natural resting point after approximately seven oscillations. We see N reduces to a new value as $N \equiv N(\mu, \omega)$, and we



Figure 5.8: a) Following the central density at gn(x = 0, t) for a damped system. Perturbation applied at the end of the imaginary time propagation. After several oscillations the density settles on a new value $gn(0,t) = 21.42\hbar\omega_x$. Parameters were $\mu = 30\hbar\omega_x$ and $g = 0.1046\hbar\omega_x l_x$. b) The particle number changing with time. c) The near-constant nature of the ratio N/n(0).

have reduced the trapping frequency. Note that for a system without noise the ratio of N/n(0) remains constant, suggesting both variables change proportionally.

5.4 Non-Equilibrium Analysis of the SGPE

5.4.1 Solitons in SGPE

In this analysis we introduce noise to the system and include particles with low thermal energy into the non-equilibrium analysis. Figure 5.9 shows a single run of the SGPE code, a), and an averaged run over 200 simulations, b). We used T = 100nK and $\mu = 30\hbar\omega_x$ to produce these graphs, and introduced the perturbation at t = 0. In the individual run, we observe that at $t = 4\omega_x^{-1}$ the soliton's lowest density is $n(x) = 12.28/g \ \hbar\omega_x$, but $n(x) = 17.49/g \ \hbar\omega_x$ in the averaged one. This difference is caused by of the random noise. Every simulation will be affected by the noise differently, as the fluctuations will interfere with the soliton's oscillations at random. So, in some runs the soliton will be damped out quicker than others. In figure 5.9 b) we are observing the most common trajectory. However, in this figure the averaged soliton appears to get wider as time goes on, which is an effect caused by the averaging. Cockburn *et*



Figure 5.9: a) A single run of the SGPE code, where we have marked the lowest density of each soliton with a black square to avoid confusion with the background noise. b) The same code averaged, the soliton is no longer as deep in this density plot due to the random nature of each individual run.

al. [49] investigated the decay rate by running a vast number of simulations, and produced a normalised histogram of the decay times for each run. We have displayed this in figure 5.10. It was discovered that the histogram could be fitted to a lognormal distribution, where the most common decay time reduced as temperature was increased. Note that the mean decay time



Figure 5.10: Normalised histogram of soliton decay times in SGPE from ref [49].

matches our results for the DGPE. This is because the noise causes the SGPE to fluctuate away from this mean value, which the DGPE does not contain.

5.4.2 Opening the Trap in the SGPE

Extending our results from section 5.3.2, we change the trapping potential in the full SGPE for sodium atoms. Figure 5.11 shows the central density, the norm and the ratio of the two, N/n(0). The quench was applied at $t = 600\omega_x^{-1}$. We see that the central density returns to its equilibrium state after the initial perturbation (from the initial system of N = 1140 particles), and after the quench the number of particles increases. This is because we lower the spacing between energy levels in the harmonic trap, after decreasing the trapping potential, thus there will be more levels under the cut-off energy. The extra particles now included in the simulation cause the central density to return to its equilibrium value. The third graph shown, the inset, shows the ratio of N/n(0). Unlike the DGPE case, this quantity increases after the quench.

Consider a slightly different analysis, where at the point of applying the perturbation we "turn off", or stop simulating, the noise and dissipation. In this scenario we cut the link with



Figure 5.11: a) Change in central density against time. b) Particle number against time. Inset: The ratio of particle number and central density.

the thermal bath after changing the trapping potential, essentially changing the code from running the SGPE, to the GPE instead. Figure 5.12 repeats the previous analysis under this regime. The central density follows a very similar pattern to that observed for the DGPE in



Figure 5.12: a) Change in central density against time. b) Particle number against time. Inset: The ratio of particle number and central density.

figure 5.8, with the new equilibrium value being lower than before the quench. This happens because we force the system into a zero temperature model, where the thermal particles cannot exist in the centre of the trap and are forced outside of the Thomas-Fermi radius. After applying the quench we force the atom number to be fixed for the new trapping potential. The most interesting part of this analysis is that the ratio between the particle number and central density has exactly the same behaviour as the full SGPE, however further analysis is required to explore this phenomena. In the full SGPE, noise damps out the oscillating behaviour quicker, which appears to be the only discernible quantity between the two.

5.4.3 Spontaneous Solitons in the Initial Quench

In this section we consider a single run from the SGPE, however instead of starting from a steady solution and analysing the effects, we instead look at the early stages of the simulation where the particle number is growing into equilibrium. Under the finite temperature regime there are high levels of fluctuations and these manifest themselves as dark solitons, in the one-dimensional case. When considering higher dimensions these fluctuations create vortices. Due to averaging these spontaneous solitons are lost in the SGPE, however they have close analogies to the early Universe. Soon after the Big Bang it has been postulated that there should have been an equal amount of matter and anti-matter. It is predicted that vortices formed through random perturbation to create clumps of matter, that later formed to be the galaxies and other stellar objects we see today, due to the Kibble-Zurek mechanism [50, 51]. In figure 5.13 we have plotted a carpet plot for the density, which clearly shows the spontaneous introduction of dark



Figure 5.13: The spontaneous introduction of solitons in the early simulation period. The parameters were chosen for Sodium atoms, with $\mu = 40\hbar\omega_x$ and T = 100nK, which corresponds to a system of about N = 1760 particles

solitons. For lower temperatures these solitons move with oscillation frequency $\omega_{\rm ds}$, with an error up to a few percent [38]. However, as the temperature increases soliton-soliton collisions have more of an effect, making it impossible to track individual solitons. We can observe that there are many solitons of different amplitudes appearing and decaying randomly throughout the simulation, the most clear of these are the solitons of highest energy at $t \approx 200\omega_x^{-1}$ and $t \approx 220\omega_x^{-1}$. We can make analogies to real systems even before a BEC is created. This type of behaviour makes the study of Bose-Einstein condensation so diverse.

Chapter 6

Conclusions and Further Work

During the course of this report we have unravelled some of the mystery behind Bose-Einstein condensation and its role in superfluids. Focusing on zero temperature weakly-interacting atomic BECs we discussed the role of the governing equation of motion for these systems, the GPE, and found solutions analytically and numerically. Within this part of the report we discussed both equilibrium and non-equilibrium dynamics of the GPE for systems that have been seen experimentally. In our analysis we examined how to perturb the trap to cause an oscillating behaviour of the condensate and we introduced and controlled dark solitons of varying speeds and depths through the medium. We also saw how two solitons interact with each other in the presence of a harmonic trap. A soliton propagating in an inhomogeneous background causes energy to escape in the form of sound waves. In a two soliton system this sound energy is transferred between the them, causing them to undergo a periodic change in amplitude. After comparing our results with Allen *et al.* [39] we found a disagreement between the two, and presented evidence for our interpretation by considering the period of oscillation for each soliton.

We also presented aspects of the theory for the SGPE, which enables us to more accurately describe a realistic system that has energy loss, random perturbation and finite temperature. Using this new theory we tested its efficacy against the already well established zero temperature model and went through the arduous process of removing the condensate from the thermal cloud. This was proceeded by a description of the non-equilibrium dynamics of the DGPE, where we ignored the random noise, to observe the effect of dissipation on the trapping potential quench and dark solitons. In both of these cases the perturbations were damped out into the background medium. We then went on to introduce random noise to the simulations, which involved connecting the system to the thermal bath. After repeating the non-equilibrium analysis for the SGPE we found that the noise caused perturbations to be washed out in the ensemble average, with the time scales appearing to change at random [49]. We also considered the spontaneous introduction of solitons in the initial quench, as predicted by the Kibble-Zurek mechanism [50, 51], which has close analogies to vortices in the early Universe.

Due to time constraints on the project there were some areas left unexplored. For example, the removal of the noise analysis performed on the trapping potential quench could have been applied to more systems, such as the Josephson effect. The Josephson effect [52] allows a current to flow indefinitely without any voltage applied across a Josephson junction, which is two superconductors coupled by a weak link. This effect has been observed in BECs by splitting it into two adjacent condensates and changing the trapping potential to allow a flow of "atomic current" between the two. Also, if time permitted, we would have compared the SGPE soliton solutions with the experiments by Becker *et al.* [53], who found that they lost the soliton after one oscillation. This is a phenomenon that could perhaps be described by the random noise of the SGPE.

Appendix A

Numerical Solution to a 1D Diffusion Equation

Here we state the tridiagonal matrix algorithm, and provide a simple example of its use. For an equation of the form

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = d_i, (A.1)$$

where $a_1 = 0$ and $c_n = 0$, we can cast this into matrix form as

$$\begin{pmatrix} b_{1} & c_{1} & & & 0 \\ a_{2} & b_{2} & c_{2} & & \\ & a_{3} & b_{3} & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ 0 & & & a_{n} & b_{n} \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \\ \vdots \\ x_{n} \end{pmatrix} = \begin{pmatrix} d_{1} \\ d_{2} \\ d_{3} \\ \vdots \\ d_{n} \end{pmatrix}.$$
 (A.2)

The solution for x_i is given by the following method, firstly we modify the coefficients as follows

$$c'_{i} = \begin{cases} \frac{c_{i}}{b_{i}}, \text{ for } i = 1, \\ \frac{c_{i}}{b_{i} - a_{i}c'_{i-1}}, \text{ for } i = 2, 3, \dots, n-1, \end{cases} \qquad d'_{i} = \begin{cases} \frac{d_{i}}{b_{i}}, \text{ for } i = 1, \\ \frac{d_{i} - a_{i}d'_{i-1}}{b_{i} - a_{i}c'_{i-1}}, \text{ for } i = 2, 3, \dots, n-1. \end{cases}$$

Then the solution is calculated through

$$x_n = d'_n, x_i = d'_i = c'_i x_{i+1}, \text{ for } i = n-1, n-2, \dots, 1.$$
 (A.3)

Here we demonstrate the accuracy of the code for a simple problem with an easily attainable analytic solution, and we will show the tridiagonal matrix algorithm used to solve it. The diffusion equation solved for the field u(x,t) with $-1 \le x \le 1$ and $t \ge 0$ is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2},\tag{A.4}$$

with boundary conditions: $u(x = \pm 1, t) = 0$ and $u(x, t = 0) = \cos(\pi x/2)$. Firstly, by using the method of separation of variables, we can find the analytical solution to this equation. From this method we obtain

$$u(x,t) = \cos\left(\frac{\pi x}{2}\right) \exp\left\{-\frac{\pi^2 t}{4}\right\}.$$
(A.5)

Using the results from section 2.3.2 we can write equation (A.4) as a Crank-Nicolson discretisation, given by

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2(\Delta x)^2} \left[(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) + (u_{i+1}^n - 2u_i^n + u_{i-1}^n) \right],$$
(A.6)

with i = 1, 2, ..., I and n = 1, 2, ..., N. If we take $r = \Delta t / [2(\Delta x)^2]$ equation (A.6) becomes

$$-ru_{i+1}^{n+1} + (1+2r)u_i^{n+1} - ru_{i-1}^{n+1} = ru_{i+1}^n + (1-2r)u_i^n + ru_{i-1}^n,$$
(A.7)

which can be cast into matrix form

$$\begin{pmatrix} 1+2r & -r & & 0 \\ -r & 1+2r & -r & & \\ & -r & 1+2r & \ddots & \\ & & \ddots & \ddots & -r \\ 0 & & & -r & 1+2r \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_1^{n+1} \\ \vdots \\ u_1^{n+1} \end{pmatrix}$$

$$= \begin{pmatrix} 1-2r & r & & 0 \\ r & 1-2r & r & & \\ & r & 1-2r & \ddots & \\ & & \ddots & \ddots & r \\ 0 & & & r & 1-2r \end{pmatrix} \begin{pmatrix} u_1^n \\ u_2^n \\ u_3^n \\ \vdots \\ u_I^n \\ \vdots \\ u_I^n \end{pmatrix},$$
(A.8)

where the right hand side is now a matrix of known variables at each time step. The tridiagonal matrix on the left hand side is invertible with the tridiagonal matrix algorithm, using $a_i = c_i = -r$ and $b_i = 1 + 2r$. With all of this information we can write the appropriate Fortran code to solve this equation. For this we took the time steps to be $\Delta t = 0.001$ s, and spatial steps to be $\Delta x = 0.01$ m. Figure A.1 shows the numerical solutions at chosen time intervals with the analytical solution overlaid, and shows how the error changes over time.



Figure A.1: a) The numerical solutions (solid lines), and overlaid analytical (dashed lines), solutions to this particular differential equation with time as indicated for each line. b) How the percentage error of the point at x = 0 differs over time.

Appendix B

Origin of Wall Solution

Here we prove the solution for the condensate wavefunction at an infinite hard wall, starting from $t = c^2 t$

$$-\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + g|\psi|^2\psi = \mu\psi.$$
(B.1)

We know the solution is real, thus $|\psi|^2 = \psi^2$, and that $n_{\infty} = \mu/g$. So we can re-write equation (B.1) as

$$-\frac{\hbar^2}{2mg}\frac{\partial^2\psi}{\partial x^2} - n_{\infty}\psi + \psi^3 = 0.$$
(B.2)

In order to solve this equation we set $\psi = \sqrt{n_{\infty}}\overline{\psi}$, then we have

$$-\frac{\hbar^2}{2mgn_{\infty}}\frac{\partial^2\bar{\psi}}{\partial x^2} - \bar{\psi} + \bar{\psi}^3 = 0.$$
(B.3)

This is similar to the ODE

$$\frac{1}{2}f'' - f + f^3 = 0, (B.4)$$

which is known to have a tanh solution. So, we will try the solution $\bar{\psi} = A \tanh Bx + C$, for constants A, B and C to be determined. Immediately we note that as the barrier is placed at x = 0 then C = 0. The second derivative of $\bar{\psi}$ can be calculated as $\bar{\psi}_{xx} = 2AB^2 [\tanh^3(Bx) - \tanh(Bx)]$. Upon substitution we have to balance the equation

$$\left[A^2 - \frac{\hbar^2}{mgn_{\infty}}B^2\right] \tanh^3(Bx) + \left[1 - \frac{\hbar^2}{mgn_{\infty}}B^2\right] \tanh(Bx) = 0,$$
(B.5)

which gives A = 1 and $B = 1/\xi$, for $\xi = \hbar/\sqrt{mn_{\infty}g}$ as the healing length. Thus substituting the equation for $\bar{\psi}$ gives

$$\psi = \psi_{\infty} \bar{\psi} = \psi_{\infty} \tanh\left(\frac{x}{\xi}\right),$$
(B.6)

as required.

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