Dipoles and Disorder:
Applications of
Hartree-Fock-Bogoliubov Theory

Sam Cormack

submitted for the degree of
Master of Science at the University of Otago.
June 2012
Abstract

We apply the Hartree-Fock-Bogoliubov-Popov (HFBP) method to two problems. The first is the phenomenon of Anderson localisation of a BEC in a two-dimensional bichromatic lattice. The second is the case of a harmonically trapped BEC with anisotropic, long-range, dipolar interactions between particles. The HFBP method allows us to calculate the condensate properties and excitation spectrum of the system at finite temperature. For the bichromatic lattice, we examine the effects of interactions and finite temperature on the localisation of the condensate. We also include a synthetic magnetic field and determine its effect. For the dipolar BEC, we examine the effect of the dipolar interactions on the condensate and thermal cloud as well as the excitation spectrum of the system. At finite temperature, we calculate the effects of both direct and exchange dipolar interactions of the thermal cloud on the condensate. The exchange interactions are numerically intensive to calculate and have been excluded from most previous studies.
Acknowledgements

Most importantly, I would like to thank my supervisor, David Hutchinson, for the help and guidance you’ve provided over the course of this research. Our meetings and emails have been invaluable. I have had many useful and interesting discussions with Joe Towers, Danny Baillie, Russell Bisset, Andrew Martin and Blair Blakie, and I thank all of you. I would especially like to thank Joe for our discussions about localisation, Danny for the use of your code, and Russell for reading this thesis.

Thank you to my parents for your love and support, and all of the opportunities I’ve had because of that. Finally, thank you to Becky for everything you do and for being such an amazing person.
Contents

1 Introduction 1

2 Background 3
  2.1 Dipolar BEC ........................................... 3
  2.2 Anderson Localisation .................................. 6

3 Theory 10
  3.1 HFB-Popov Overview .................................. 10
  3.2 Lattice HFBP ........................................... 14
    3.2.1 Bose Hubbard Model ................................. 16
    3.2.2 Lattice Equations ................................ 17
    3.2.3 Synthetic Magnetic Field ......................... 18
  3.3 Dipolar HFBP .......................................... 19

4 Numerical Methods 23
  4.1 Dipole Implementation ................................. 23
    4.1.1 2D GP Equation .................................. 24
    4.1.2 BdG Equations ..................................... 26
    4.1.3 Dipolar Interaction Potential ..................... 28
    4.1.4 Hankel Transforms ................................ 29
  4.2 Lattice Implementation ................................ 30

5 Localisation Results 31
  5.1 Units and Parameters .................................. 31
  5.2 Localisation in 2D ..................................... 31
  5.3 Interaction Effects .................................... 34
  5.4 Finite Temperature Effects ............................ 35
  5.5 Synthetic Magnetic Field .............................. 37

6 Dipolar BEC Results 41
  6.1 Units and Parameters .................................. 41
  6.2 Density Profiles ...................................... 42
6.3 Effective Dipolar Potential ........................................... 44
6.4 Excitations ................................................................. 45

7 Thermal Dipolar Exchange .............................................. 50
7.1 Calculating the thermal exchange term ......................... 50
7.2 Excitations ................................................................. 54

8 Conclusions ..................................................................... 56
8.1 Anderson Localisation .................................................... 56
8.2 Dipolar BEC ................................................................. 57

A Derivation of Exchange Term in 2D .................................. 59
Chapter 1

Introduction

Since the creation of the first Bose-Einstein condensates (BEC) from dilute gases, there has been an incredible proliferation of different systems in which Bose-Einstein condensation has been achieved. Various atomic species have been condensed, such as $^{87}$Rb [1], $^{23}$Na [2], $^7$Li [3], $^3$H [4], $^{85}$Rb [5], $^4$He [6], $^{41}$K [7], $^{133}$Cs [8], $^{52}$Cr [9] and more recently, $^{164}$Dy [10] and $^{168}$Er [11]. Bose-Einstein condensates have also been created using a variety of trap geometries. Early condensates were created using magneto-optical traps which provide an axially symmetric, harmonic potential [1]. Quasi-one dimensional and two dimensional condensates have been produced by tightly confining the system in one or two directions [12, 13]. Condensates in a lattice geometry can also be created by applying an optical lattice [14, 15]. The range of variations of BECs provides a rich range of behaviour to explore.

In this work we will explore the properties of two systems where Bose-Einstein condensates are present. First we will look at atoms in a two-dimensional bichromatic lattice and examine the phenomenon of Anderson localisation. In this system, the atoms are cooled to form a BEC and trapped in a 2-D optical lattice. A second optical lattice is applied to the system and this lattice has a wavelength which is incommensurate with the first. This offsets the energies of each of the main lattice sites in a pseudo-random way, introducing disorder into the system. This disorder inhibits the transport of particles through the lattice and this is known as Anderson localisation. This localisation of a condensate has been observed in a recent experiment using a one-dimensional bichromatic lattice [16].

Using the same tools, we will also examine a harmonically trapped BEC with dipolar interactions between particles. In contrast to the usual contact interactions which are used in most models, dipolar interactions are long-range and anisotropic, leading to various interesting effects. Interest in dipolar BECs has been spurred by successful Bose-Einstein condensation of atoms with strong magnetic moments ($^{52}$Cr, $^{164}$Dy and $^{168}$Er). In chapter 2 we will give some more background on the theoretical and experimental work that has been done on these systems and on An-
In chapter 3 we will present the method used to study both of our systems. This is the Hartree-Fock-Bogoliubov method with the Popov approximation (HFBP). This method allows us to calculate the properties of the condensate, and the excitation spectrum, at finite temperature. We will give an outline of the general theory and then apply it to the bichromatic lattice and the dipolar BEC, obtaining the HFBP equations for each case. In chapter 4 we will discuss some of the technical issues that occur when solving these equations numerically. The solution method for the HFBP equations of the bichromatic lattice is relatively straightforward, however, the dipolar BEC calculations present a number of difficulties which must be dealt with.

We will present our results on localisation in the bichromatic lattice in chapter 5. We show the onset of localisation for the simplest, non-interacting case first. We then explore the effects of introducing interactions between particles and increasing the temperature of the system. We also investigate what happens when apply a synthetic magnetic field to the system. Although neutral atoms are used to produce Bose-Einstein condensates, we can imitate the effect of magnetic fields on charged particles by special laser configurations.

The results of our calculations on the dipolar BEC are presented in chapters 6 and 7. When solving the HFBP equations for this system, one term in particular presents a significant numerical challenge: the thermal dipolar exchange term. This term has been excluded in most previous studies as it is much more difficult to calculate than the rest of the equations and it was thought to have only a small effect. We too exclude this term in chapter 6 and calculate the properties of the condensate and thermal cloud as well as the excitation spectrum for the dipolar BEC. In chapter 7 we perform calculations including this term in order to determine how much of an effect it has.
Chapter 2

Background

Bose-Einstein condensates made from different atomic species can have quite different behaviour. The atomic mass has a direct effect on the condensation temperature while the energy level structure affects the way the atoms may be trapped and cooled. Some of the most interesting differences between BECs of different atomic species results from differences in interparticle interactions. The standard method for treating interactions in a BEC is to assume there are only short-range interactions governed by the $s$-wave scattering length. This approach works well for atoms such as rubidium and lithium. The scattering length for $^{87}$Rb is positive, meaning the short-range interaction is repulsive. On the other hand the scattering length for $^{7}$Li is negative so it has an attractive short-range interaction. This will cause a homogeneous BEC of $^{7}$Li to be unstable [17]. A trapped condensate will, however, be stable [18, 19], provided it is not too large. The strength and sign of the interaction affects the shape of the density profile with repulsive interactions tending to spread the condensate out and attractive interactions pulling the condensate in and increasing the central density [18]. The size and sign of the effective scattering length in a BEC can now be tuned by using Feshbach resonances [20, 5].

2.1 Dipolar BEC

We usually consider atoms in a BEC to interact via a van der Waals potential which drops off like $1/r^6$ at large distances. It can be shown that for such a potential, the low energy scattering is dominated by the $s$-wave scattering [21]. At temperatures low enough for a BEC to form, only low energy scattering occurs so we can safely replace the actual interaction potential with a pseudopotential which reproduces the $s$-wave scattering. This pseudopotential is usually a delta function with the same $s$-wave scattering length. We cannot always assume that interactions between particles in a BEC are short-range only however. Chromium, dysprosium and erbium
have significant magnetic dipole moments ($6\mu_B$ for $^{52}\text{Cr}$ [9], $10\mu_B$ for $^{164}\text{Dy}$ [10] and $7\mu_B$ for $^{168}\text{Er}$ [11], where $\mu_B$ is the Bohr magneton). The dipolar interaction potential drops off like $1/r^3$ for large distances. In this case, all of the higher order partial waves contribute to the scattering at low energy [21]. We therefore cannot replace the true potential with a short-range pseudopotential. When atoms with significant magnetic dipole moments are Bose-condensed we must take into account the long-range nature of the dipolar interaction between atoms and this will give rise to new and interesting behaviour.

The theoretical approach to Bose-Einstein condensation commonly starts at the Gross-Pitaevskii equation (GPE). This equation applies at zero temperature and, for a BEC with short-range interactions, is given by [22]

$$i\hbar \frac{\partial}{\partial t} \Phi(x, t) = \left( -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{ext}}(x) + g|\Phi(x, t)|^2 \right) \Phi(x, t)$$

(2.1)

where $\Phi(x, t)$ is the condensate wavefunction, $V_{\text{ext}}(x)$ is the external potential and $g = 4\pi\hbar^2 a/M$ characterises the interaction strength for a scattering length, $a$. This equation is the simplest theoretical tool for investigating inhomogeneous Bose-Einstein condensates.

The GPE can also be derived for the case of dipolar interactions between particles. The simplest case to handle numerically is a cylindrically symmetric system. This occurs when the trap is cylindrically symmetric about the $z$ axis and the dipole moments of the atoms are also aligned along this axis. This can be achieved by applying an external magnetic field (for atoms with a magnetic dipole moment). When this configuration is used, interactions along the symmetry axis of the trap will be attractive, while they will be repulsive in the plane perpendicular to the axis. In this case the GPE reads

$$i\hbar \frac{\partial}{\partial t} \Phi(x, t) = \left( -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{ext}}(x) + g|\Phi(x, t)|^2 + \int d\mathbf{x}' V_{\text{dd}}(\mathbf{x}' - \mathbf{x})|\Phi(\mathbf{x}', t)|^2 \right) \Phi(x, t)$$

(2.2)

where $V_{\text{dd}}(x)$ is the dipolar interaction potential for $z$-aligned dipoles given by

$$V_{\text{dd}}(\mathbf{x}) = d^2 \frac{1 - 3\cos^2 \theta}{|\mathbf{x}|^3}$$

(2.3)

where $d$ is the dipole strength, and $\theta$ is the angle between the dipole moment and the separation vector, $\mathbf{x}$. A cylindrically symmetric potential will have the form,

$$V_{\text{ext}}(\mathbf{x}) = \frac{1}{2}M(\omega_\rho^2 \rho^2 + \omega_z^2 z^2)$$

(2.4)

where $\rho$ and $z$ are standard cylindrical coordinates and $\omega_\rho$ and $\omega_z$ are the corre-
Figure 2.1: The arrows represent dipoles aligned along the $z$ axis of a trap. Dipoles which are side-by-side, such as the two on left, will experience repulsion. Dipoles which are head-to-tail, such as those on the right will experience attraction.

responding trapping frequencies. We can define $\lambda = \omega_z/\omega_\rho$ as the aspect ratio of the trap. Traps with $\lambda > 1$ are more strongly confined in the axial direction and we call these *disk-shaped* or *pancake* traps. Those with $\lambda < 1$ are more strongly confined in the radial direction and these are referred to as *cigar-shaped*.

Equation (2.2) was first used by Yi and You [23], and Góral et al. [24] to calculate the zero temperature density profiles for dipolar BECs. Yi and You looked at the case of a pancake trap with $\lambda = \sqrt{8}$. They found that increasing the strength of dipolar interaction caused the condensate to contract in the radial direction and expand in the axial direction while the peak density increased. Meanwhile, Góral et al. compared the density profile of the dipolar BEC to an equivalent BEC with only contact interactions. They found that for a pancake trap, the dipolar BEC was larger in the radial direction. For a cigar trap, the condensate was smaller in both the radial and axial direction. These studies showed that the anisotropic nature of the dipole interaction had significant effects on the shape of a condensate. The dipolar GPE was also used in the work of Santos et al. [25] to study the stability of a dipolar condensate with no contact interactions.

The natural next direction is to look at the excitation spectrum of the system. Again, this problem was first approached by Yi and You [26], and Góral and Santos [27]. Both groups used a time-dependent, Gaussian variational ansatz in the GPE to calculate the energies of the three lowest excitations. Both groups also compare these results to numerical solutions of the time-dependent GPE. They do this by starting with the ground state wavefunction and applying a time-varying potential to excite oscillations. Fourier analysis can then be applied to the changing conden-
sate width to determine the oscillation frequency components. Both groups find good agreement between variational and numerical results when the dipolar interaction is relatively weak, however, Góral and Santos find that this agreement breaks down when the dipolar interactions start to drive the condensate towards collapse.

The standard approach to determining the excitation energies of a BEC is to use Bogoliubov theory \[ (22) \]. This approach was used by Ronen, Bortolotti and Bohn \[ (28) \] to calculate the excitations of the dipolar BEC. The Bogoliubov method was not used by previous studies \[ (26, 27) \] due to the numerical difficulty in solving the equations. Ronen et al. overcame this difficulty by utilising both the cylindrical symmetry of the problem and the convenient form of the dipolar interaction term in momentum space. This method will be discussed further in chapter 3. The authors calculated the excitation energies for varying dipole strengths in a number of trap geometries. They also calculated the quantum depletion of the condensate.

In another article, Ronen, Bortolotti and Bohn \[ (29) \] examined the stability of the dipolar gas. They found that, contrary to a previous study \[ (25) \], the condensate is unstable for any trap geometry if enough particles are added. They also found that for highly pancake traps with particular aspect ratios (e.g. \( \lambda \approx 7 \)), the condensate develops a biconcave, or red blood cell-like, shape as it approaches instability. Ronen and Bohn \[ (30) \] extended their method to condensates at non-zero temperature using Hartree-Fock-Bogoliubov theory with the Popov approximation \[ (31, 32) \]. The excitation energies and condensate fraction are calculated as a function of temperature. They also found that biconcave condensates still existed at finite temperature. In this work Ronen and Bohn did not include the effects of dipolar exchange interactions of the thermal cloud on the condensate as these effects are computationally intensive to calculate. We have included this interaction in our work to determine what effect it has.

Another interesting aspect of dipolar condensates is the existence of roton excitations usually associated with superfluid helium \[ (33) \]. Rotons are most easily detected in a homogeneous system where excitation energies are naturally written as a function of momentum. A roton-maxon excitation spectrum is one which contains a local minimum in energy with respect to momentum. Rotons correspond to excitations near this minimum. A homogeneous 3D purely dipolar condensate is not stable so the first predictions of roton excitations in a dipolar BEC were for quasi-1D \[ (34) \] and quasi-2D \[ (35) \] systems.

### 2.2 Anderson Localisation

The ability to create Bose-Einstein condensates in lattice geometries gives us the opportunity to study the phenomenon of Anderson localisation \[ (36) \]. Anderson was
investigating the transport properties of particles in a lattice, such as electrons in a metal. In a translationally invariant lattice, we can think of transport as being via waves which travel freely through the lattice. If there are impurities in the lattice, these waves may scatter off them [37]. In some cases, however, it is better to think of particles localised to lattice sites which travel by hopping between sites. Anderson showed that when enough disorder is introduced, for example by postulating that the energies of particles at different lattice sites are distributed randomly, transport can be completely inhibited. This is what we now call Anderson localisation and it is characterised by exponential decay of the particles’ wavefunction with distance.

For a particle at a lattice site centred at \( \mathbf{x}_0 \) this means the wavefunction will behave like [37]

\[
|\psi(\mathbf{x})| \sim \exp\left(-|\mathbf{x} - \mathbf{x}_0|/l\right) \tag{2.5}
\]

where \( l \) is the length scale of the localisation.

In a solid, localised electron states will mean that the material is insulating, while extended states imply it is a conductor. For a given amount of disorder, the transition between an insulator and a conductor occurs for a critical electron density or, equivalently, a critical Fermi energy, \( E_c \). If the Fermi energy is less than \( E_c \) the electron states will be localised and the material is an insulator. In a one-dimensional lattice there is no transition and all states are localised for any amount of disorder [38, 39]. The nature of the transition in two and three dimensions was controversial for a long time. Mott [40] argued that the transition was discontinuous, i.e. that there is some minimum, non-zero, conductivity at the critical Fermi energy. Licciardello and Thouless [41] predicted that this minimum conductivity would be universal in two dimensions. At about the same time, Thouless and others developed a scaling theory of localisation [42, 43, 44, 45]. The scaling theory predicted a continuous transition between insulating and conducting states, contradicting Mott’s prediction of a minimum conductivity. Numerical work by MacKinnon and Kramer [46] supports the prediction of a continuous transition in three dimensions.

It is difficult to observe Anderson localisation directly in systems of electrons. The Coulomb interaction complicates the situation considerably [37] and there is usually limited control over the parameters of the system. An alternative system for observing Anderson localisation was proposed in which photons are localised by a disordered medium [47]. This has the advantage that photons do not interact with each other, so the complications introduced by interactions for electrons are avoided. A number of experiments have now reported observation of Anderson localisation in such systems [48, 49, 50, 51, 52].

Recently, two groups have reported the observation of Anderson localisation in Bose-Einstein condensates. The experiment from the group of Bouyer and Aspect
[53] used the potential created by laser speckle to introduce disorder. The BEC was produced in a one-dimensional optical waveguide. It is initially trapped along the longitudinal direction and when it is released in the absence of disorder, it expands freely. When the laser speckle is applied to the released cloud, the expansion is halted and the density has an exponential decay in the wings, as expected for Anderson localisation. Inguscio’s group [16] used a different different approach to producing the disorder needed to explore localisation. The BEC is created in a one-dimensional optical lattice and disorder is introduced by adding a second incommensurate lattice, creating a bichromatic lattice. Because the second lattice potential is incommensurate with the first, it shifts the energies of the main lattice sites in a pseudo-random way. The scattering length of the atoms is reduced by means of a Feshbach resonance in an attempt to minimise interaction effects. This group also observed exponentially localised states. Bose-Einstein condensates provide an excellent testing ground for Anderson localisation as both the trapping geometry and strength of interactions can be controlled. Anderson localisation has also been observed in ultracold fermion systems. Brian DeMarco’s group used laser speckle to introduce disorder into a system of $^{40}$K atoms below the Fermi temperature [54]. They observed Anderson localisation in a fully three-dimensional system in contrast to the essentially one-dimensional systems used in the BEC localisation experiments.

The BEC in a 1D bichromatic lattice is an example of the Aubry-André or Harper model [55]. It shows a sharp transition between localised and extended states when interactions are absent. This transition is analogous to the usual Anderson transition in systems of higher dimension. The transition can occur here in a one-dimensional system as the disorder is not fully random [56]. The introduction of interactions complicates the situation and makes it more difficult to observe disorder-induced localisation. A number of studies have considered the effect of interactions on the Aubry-André model [57, 58, 59, 60]. Larcher, Dalfovo and Modugno [60] identify two separate effects of the interactions: self-trapping and delocalisation. Delocalisation is simply the breaking of disorder-induced localisation when interactions are present. If interactions are strong enough, then the BEC will start to spread for disorder strengths where it would have been localised without interactions.

Self-trapping refers to a form of localisation caused by the initial interaction energy in the BEC. It is independent of any disorder in the system and can occur in a periodic lattice. Self-trapping can be understood in terms of energy conservation.
The Hamiltonian of the Aubry-Andrè model with contact interactions is

\[ H = \sum_j V_j |\psi_j|^2 - J(\psi_{j+1}\psi_j^* + \psi_{j+1}^*\psi_j) + \frac{U}{2} |\psi_j|^4 \]  

(2.6)

where \( \psi_j \) is the amplitude for finding a particle at the primary lattice site \( j \), \( V_j \) is the potential from the secondary lattice, \( J \) measures the amount of tunnelling between sites and \( U \) is the interaction strength. The energy in the terms quadratic in \( \psi_j \) gives the potential and kinetic energy and there is a maximum amount of energy which can be accounted for by these terms. If the interaction strength is strong enough and the initial state is localised, the interaction strength can be much greater than this energy. In this case, the initial state cannot spread as it cannot give up its initial interaction energy to kinetic energy. Experiments which aim to observe disorder-induced localisation must therefore be careful to distinguish it from self-trapping due to interactions. We will examine the localisation of a BEC in a two dimensional bichromatic lattice. This will allow us to introduce synthetic magnetic fields and determine their effect on localisation. Synthetic magnetic fields would have no effect on a one dimensional lattice. In order to study effect of finite temperatures on the localisation, we use the time-independent HFBP formalism. Using this formalism, we cannot directly observe the time-dependent localisation of the condensate, however, we can observe when the condensate solution becomes exponentially localised on small scales independent of the boundary conditions. This signals the onset of localisation.
Chapter 3

Theory

In this chapter we will outline the general Hartree-Fock-Bogoliubov method with the Popov approximation which will be used for both the bichromatic lattice problem and the dipolar BEC. This method allows us to examine the properties of the condensate at finite temperature. We will then show how the method can be applied to both problems and give the resulting equations.

3.1 HFB-Popov Overview

We would like to study the behaviour of systems of bosons at temperatures low enough for a condensate to be present. Conceptually, the Hartree-Fock-Bogoliubov method consists of splitting the system of interest into a condensate and a thermal cloud. The condensate is governed by a slightly altered version of the Gross-Pitaevskii equation. The properties of the thermal cloud are determined by calculating the excited states of the system and populating them with the Bose distribution. The equations for the condensate and excited states are coupled and we look for a self-consistent solution. The derivation of these equations will be outlined in this section. We present a similar derivation to that given by Hutchinson et al. [61] which was for contact interactions.

We work in the grand canonical ensemble where the number of particles in the system is determined by the chemical potential, \( \mu \). Thermodynamic quantities may be calculated from the partition function,

\[ Z = \text{Tr} \, e^{-\beta K} \quad (3.1) \]

where the grand canonical Hamiltonian, \( \hat{K} \), is defined by \( \hat{K} = \hat{H} - \mu \hat{N} \). The general
Hamiltonian for an interacting many-body system, using field operators, is

\[
\hat{K} = \int \! d\mathbf{x} \, \Psi^\dagger(\mathbf{x}) \left( \hat{H}_{\text{sp}} - \mu \right) \Psi(\mathbf{x}) + \frac{1}{2} \int \! d\mathbf{x} \, d\mathbf{x'} \, \Psi^\dagger(\mathbf{x}) \Psi^\dagger(\mathbf{x'}) V(\mathbf{x'} - \mathbf{x}) \Psi(\mathbf{x}) \Psi(\mathbf{x'}) \tag{3.2}
\]

where the single particle Hamiltonian, \( \hat{H}_{\text{sp}} \), is given by

\[
\hat{H}_{\text{sp}} = -\frac{\hbar^2}{2M} \nabla^2 + V_{\text{ext}}, \tag{3.3}
\]

and \( V(\mathbf{x}) \) is the interaction potential.

The first step is to expand the field operators in an orthonormal, single particle basis,

\[
\Psi(\mathbf{x}) = \phi_0(\mathbf{x}) \hat{a}_0 + \sum_i \phi_i(\mathbf{x}) \hat{a}_i. \tag{3.4}
\]

We do not define the basis yet, as the most convenient one to choose will become clear later. The function \( \phi_0(\mathbf{x}) \) is the ground state wavefunction and, as we will be considering temperatures at which condensation occurs, it will be highly occupied. This assumption allows us to replace the operator \( \hat{a}_0 \) with a c-number, \( \sqrt{N_0} \), where \( N_0 \) is the number of atoms in the condensate. One way of looking at this is that we are treating the ground state as a coherent state. We then define the condensate wavefunction,

\[
\Phi(\mathbf{x}) = \sqrt{N_0} \phi_0(\mathbf{x}) \tag{3.5}
\]

and the fluctuation operator,

\[
\psi(\mathbf{x}) = \sum_{i=1} \phi_i(\mathbf{x}) \hat{a}_i \tag{3.6}
\]

so that equation (3.4) can be rewritten as

\[
\Psi(\mathbf{x}) = \Phi(\mathbf{x}) + \psi(\mathbf{x}). \tag{3.7}
\]

By substituting (3.7) into the Hamiltonian (3.2), we obtain an expression for the Hamiltonian which may be separated into terms with different numbers of \( \psi(\mathbf{x}) \). The zeroth-order term, in which \( \psi(\mathbf{x}) \) does not appear, is

\[
\hat{K}_0 = \int \! d\mathbf{x} \, \Phi^\dagger(\mathbf{x}) \left( \hat{H}_{\text{sp}} - \mu \right) \Phi(\mathbf{x}) + \frac{1}{2} \int \! d\mathbf{x} \, d\mathbf{x'} \, |\Phi(\mathbf{x'})|^2 V(\mathbf{x'} - \mathbf{x}) |\Phi(\mathbf{x})|^2. \tag{3.8}
\]

The next term, linear in \( \psi(\mathbf{x}) \), is

\[
\hat{K}_1 = \int \! d\mathbf{x} \, \psi^\dagger(\mathbf{x}) (\hat{h}_{\text{GP}} - \mu) \Phi(\mathbf{x}) + \text{h.c.} \tag{3.9}
\]
where h.c. stands for Hermitian conjugate and the operator $\hat{h}_{GP}$ is given by

$$\hat{h}_{GP} = \hat{H}_{sp} + \int d\mathbf{x}' V(\mathbf{x}' - \mathbf{x})|\Phi(\mathbf{x}')|^2$$  \hspace{1cm} (3.10)$$

At this stage we can recover the Gross-Pitaevskii equation by using the variational principle and ensuring the Hamiltonian is stationary with respect to first order variation in $\psi(\mathbf{x})$. This means that $\Phi(\mathbf{x})$ must satisfy

$$\hat{h}_{GP}\Phi(\mathbf{x}) = \mu \Phi(\mathbf{x}).$$  \hspace{1cm} (3.11)$$

which is the GPE for an arbitrary interaction potential.

The second order term is

$$\hat{K}_2 = \int d\mathbf{x} \psi(\mathbf{x}) \hat{L}_0 \psi(\mathbf{x}) + \left( \frac{1}{2} \int d\mathbf{x} \left[ \hat{M} \psi(\mathbf{x}) \right] \right) \psi(\mathbf{x}) + \text{h.c.}$$  \hspace{1cm} (3.12)$$

where

$$\hat{L}_0 = \hat{h}_{GP} - \mu + \hat{M},$$  \hspace{1cm} (3.13)$$

and the operator $\hat{M}$ is defined by

$$\hat{M} \psi(\mathbf{x}) = \Phi(\mathbf{x}) \int d\mathbf{x}' \Phi(\mathbf{x}') V(\mathbf{x}' - \mathbf{x}) \psi(\mathbf{x}')$$  \hspace{1cm} (3.14)$$

for arbitrary $\psi(\mathbf{x})$. If we were to diagonalise $\hat{K}_2$ now, we would obtain the Bogoliubov-de Gennes (BdG) equations for the excitations. This is called the Bogoliubov approximation. This is a zero temperature theory and the calculated excitations are not thermally populated. There will however be a small depletion of the condensate due to interactions.

To go beyond the Bogoliubov theory we must include the cubic and quartic terms. These terms are treated in an approximate way by using a mean-field factorisation. For example, a cubic term of the form $\psi(\mathbf{x}) \psi(\mathbf{x}') \psi(\mathbf{x})$ is approximated by

$$\psi(\mathbf{x}) \psi(\mathbf{x}') \psi(\mathbf{x}) \approx \langle \psi(\mathbf{x}) \psi(\mathbf{x}') \psi(\mathbf{x}) \rangle \psi(\mathbf{x}) + \langle \psi(\mathbf{x}) \psi(\mathbf{x}) \psi(\mathbf{x}) \rangle \psi(\mathbf{x}') + \langle \psi(\mathbf{x}') \psi(\mathbf{x}) \psi(\mathbf{x}) \rangle \psi(\mathbf{x})$$  \hspace{1cm} (3.15)$$

Other terms are approximated in the same way by taking the expectation value of each pair of operators and multiplying this by the remaining operators in the product. These terms are then summed. To simplify the notation we introduce the quan-
\begin{align}
\tilde{n}(x', x) &\equiv \langle \tilde{\psi}^\dagger(x') \tilde{\psi}(x) \rangle \quad (3.16) \\
\tilde{n}(x) &\equiv \tilde{n}(x, x) \quad (3.17) \\
m(x', x) &\equiv \langle \tilde{\psi}(x') \tilde{\psi}(x) \rangle \quad (3.18)
\end{align}

\(\tilde{n}(x', x)\) is the non-condensate one body density matrix, \(\tilde{n}(x)\) is the non-condensate density and \(m(x', x)\) is the anomalous density matrix. We disregard terms involving \(m(x', x)\) which leads to the Popov approximation. We do this to ensure the excitation spectrum is gapless as required by Goldstone’s theorem [62].

When these approximations are made, the cubic term gives a contribution to \(\hat{K}_1\) which amounts to replacing \(\hat{h}_{GP}\) with \(\hat{h}_0\) where \(\hat{h}_0\) is defined by

\[
\hat{h}_0 \psi(x) = \left[ \hat{H}_{sp} + \int \! dx' \, V(x' - x) \left( |\Phi(x')|^2 + \tilde{n}(x') \right) \right] \psi(x) + \int \! dx' \, \tilde{n}(x', x) V(x' - x) \psi(x')
\]

(3.19)

The quartic term is approximated to a quadratic term which is again taken into account by replacing \(\hat{h}_{GP}\) by \(\hat{h}_0\). \(\hat{K}_2\) will have the same form as in equation (3.12) but with \(\hat{L}_0\) replaced by

\[
\hat{L} = \hat{h}_0 - \mu + \hat{M}.
\]

(3.20)

Now, by applying the variational principle, we obtain the generalised Gross-Pitaevskii equation, applicable to a condensate interacting with a thermal cloud

\[
\hat{h}_0 \phi_0(x) = \mu \phi_0(x)
\]

(3.21)

The interaction term in square brackets in equation (3.19), involving both the condensate density, \(|\Phi(x')|^2\), and the non-condensate density, \(\tilde{n}(x')\), is called the direct or Hartree interaction. This name comes about due to Hartree’s original mean-field theory for electrons where the wavefunction is postulated to be a product of single-particle wavefunctions. It is easily interpreted as the average potential experienced by each particle due to all the other particles. The final term in equation (3.19) is called the exchange or Fock term. It involves the non-condensate one body density matrix. The name comes from Fock’s addition to Hartree’s theory where the trial wavefunction is symmetrised (or antisymmetrised). The exchange term appears due to the field operator commutation relations and thus ultimately from the Bose symmetry of the system.

We would like to determine the excited mode amplitudes and energies, and, via these, the non-condensate quantities. To do this we must diagonalise the remaining
\( K_2 \) term in the Hamiltonian. This is done via the standard Bogoliubov method. The fluctuation operator is written in terms of new amplitudes and operators,

\[
\hat{\psi}(\mathbf{x}) = \sum_i \left[ u_i(\mathbf{x}) \hat{\alpha}_i - v_i(\mathbf{x}) \hat{\alpha}_i^\dagger \right]
\]

where the operators \( \hat{\alpha}_i \) obey Bose commutation relations. When this expression is substituted into the expression (3.12), \( \hat{K}_2 \) will be diagonalised if the amplitudes \( u_i \) and \( v_i \) obey the Bogoliubov-de Gennes (BdG) equations

\[
\begin{align*}
\hat{L} u_i(\mathbf{x}) - \hat{M} v_i(\mathbf{x}) &= E_i u_i(\mathbf{x}) \\
\hat{L}^* v_i(\mathbf{x}) - \hat{M}^* u_i(\mathbf{x}) &= -E_i v_i(\mathbf{x})
\end{align*}
\]

where the eigenvalues, \( E_i \), are interpreted as the energies of the excitations. The commutation relation for the original field operator, \( \hat{\psi}(\mathbf{x}) \), leads to the following orthonormality conditions for the amplitudes,

\[
\int d\mathbf{x} \left( u_i^\dagger(\mathbf{x}) u_j(\mathbf{x}) - v_i^\dagger(\mathbf{x}) v_j(\mathbf{x}) \right) = \delta_{ij}
\]

The thermal expectation value of the quasiparticle expectation number can be shown to have the form of a Bose distribution [32]

\[
\langle \hat{\alpha}_i^\dagger \hat{\alpha}_i \rangle = \frac{1}{e^{\beta E_i} - 1} \equiv N_{BE}(E_i)
\]

Using this, we can express the non-condensate one body density matrix in terms of the quasiparticle amplitudes by substituting equation (3.22) into the definition of \( \tilde{n}(\mathbf{x}', \mathbf{x}) \) giving

\[
\tilde{n}(\mathbf{x}', \mathbf{x}) = \sum_i \left\{ [u_i^*(\mathbf{x}') u_i(\mathbf{x}) + v_i(\mathbf{x}') v_i^*(\mathbf{x})] N_{BE}(E_i) + v_i(\mathbf{x}') v_i^*(\mathbf{x}) \right\}
\]

From this we can easily obtain the non-condensate density, \( \tilde{n}(\mathbf{x}) \), by setting \( \mathbf{x}' = \mathbf{x} \). These quantities can then be fed back into the generalised GPE, (3.21), and we can solve the full set of equations self-consistently.

\subsection*{3.2 Lattice HFBP}

We will now apply the HFBP formalism to the first of our two systems of interest. We will be looking at atoms trapped in a 2D lattice with disorder introduced by weaker incommensurate lattice potentials. The lattice potential is produced by creating an interference pattern from multiple lasers. Trapping occurs by the same
mechanism as a dipole trap, that is, the AC Stark Shift \[63\]. In this type of trap, an atom’s energy depends on the intensity of the light field at its position, so an interference pattern creates a lattice trap.

For the lattice application of HFBP, we will consider only contact interactions. This involves replacing the full inter-particle interaction potential with a pseudo-potential, \(V(x) = g\delta(x)\), which gives the same low-energy scattering properties [22]. This allows us to simplify the interaction term in equation (3.2) to

\[
\frac{g}{2} \int dx \hat{\Psi}^{\dagger}(x) \hat{\Psi}^{\dagger}(x) \hat{\Psi}(x) \hat{\Psi}(x).
\]

The Hamilton for the 2D disordered lattice system is therefore

\[
\hat{H} = \int dx \hat{\Psi}^{\dagger}(x) \left( -\frac{\hbar^2}{2M} \nabla^2 + V_L(x) + V_{\text{dis}}(x) \right) \hat{\Psi}(x) + \frac{g}{2} \int dx \hat{\Psi}^{\dagger}(x) \hat{\Psi}^{\dagger}(x) \hat{\Psi}(x) \hat{\Psi}(x)
\]

(3.27)

where \(M\) is the atomic mass, \(V_L(x)\) is the strong primary lattice potential and \(V_{\text{dis}}(x)\) is the weaker secondary lattice potential which introduces disorder. The lattice potential is given by

\[
V_L(x) = V_o (\sin^2(2\pi x/\lambda_L) + \sin^2(2\pi y/\lambda_L)),
\]

(3.28)

where \(V_o\) is the “depth” of the lattice and \(\lambda_L\) is its wavelength. For the disorder potential we use a lattice with a wavelength incommensurate with the main lattice. This gives a potential,

\[
V_{\text{dis}}(x) = s \left( \cos^2 \left( \frac{2\pi}{\lambda_a}(x + \delta x) \right) + \cos^2 \left( \frac{2\pi}{\lambda_a}(y + \delta y) \right) \right),
\]

(3.29)

where \(s\) is the “depth” of the disorder potential, \(\delta x\) and \(\delta y\) are phase offsets, and \(\lambda_a\) is the wavelength of the secondary lattice.

We will be using infinite potential, or reflecting, boundary conditions. The ground state of the system when there is no disorder will therefore be that of an infinite square well in two dimensions. The transition from extended states to localised states is signalled by the change in ground state from the square well solution to an exponentially localised solution. We have not used periodic boundary conditions as the secondary lattice will never have the same periodicity as the primary lattice (by construction). Periodic boundary conditions will therefore still be partially reflecting due to the sudden change in potential at the boundary.
3.2.1 Bose Hubbard Model

In studying localisation effects for bosons in a lattice potential, we will use the Bose-Hubbard Hamiltonian, appropriate in the tight-binding limit. This is given by

\[ \hat{H}_{BH} = \sum_i \hat{n}_i \varepsilon_i - J \sum_{<ij>} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \]  

(3.30)

where the creation operator \( \hat{a}_i^\dagger \) adds a particle to the \( i \)th lattice site and the lattice site number operator is \( \hat{n}_i \equiv \hat{a}_i^\dagger \hat{a}_i \). The constants \( \varepsilon_i, J \) and \( U \) are the onsite energy, tunnelling amplitude, and onsite interaction strength respectively. These will be defined shortly. The summation over \( <ij> \) means that we should sum only nearest neighbour pairs of creation and destruction operators.

The Bose-Hubbard Hamiltonian may be derived from the Hamiltonian, (3.27), by expanding the field operators in the set of Wannier functions localised at each lattice site. In the tight binding limit, where the lattice potential is deep, atoms will not be excited to higher vibrational states at each site. We can therefore use only the lowest band Wannier functions. The expansion has the form \( \hat{\psi}(x) = \sum_i \hat{a}_i w(x - x_i) \), where \( w(x) \) is the lowest band Wannier function centred at the origin. The \( x_i \) are the positions of the lattice sites. The lattice is square with a lattice constant of \( \lambda_L/2 \).

Using this expansion in equation (3.2) leads to the Bose-Hubbard Hamiltonian.

The first term in equation (3.30) represents the kinetic and potential energy of the atoms at each lattice site. In the absence of the disorder potential, every lattice site would be identical and this term would provide a constant offset to the Hamiltonian which can be ignored. We therefore include only the effect of the disorder potential, \( V_{\text{dis}}(x) \) on the onsite energy, \( \varepsilon_i \),

\[ \varepsilon_i = \int dx \ w^*(x - x_i) V_{\text{dis}}(x) w(x - x_i) \]  

(3.31)

If there is an external trapping potential in addition to the lattice potentials it also needs to be included in the onsite energy. The onsite energy can be put into the form [56],

\[ \varepsilon_{jk} = \Delta(\cos(2\pi a j + \delta\varphi_x) + \cos(2\pi a k + \delta\varphi_y)), \]  

(3.32)

where \( j \) and \( k \) are the lattice indices for the \( x \) and \( y \) directions respectively, \( a = \lambda_L/\lambda_\alpha \), and \( \delta\varphi_x \) and \( \delta\varphi_y \) are phase offsets. The parameter \( \Delta \) is referred to as the disorder strength and is given by

\[ \Delta = \frac{s}{2} \int d\xi \ d\zeta \ \cos(2\alpha\xi)|w(\xi, \zeta)|^2 \]  

(3.33)

where \( \xi = 2\pi x/\lambda_L \) and \( \zeta = 2\pi y/\lambda_L \).
The energy eigenstates of the primary lattice are Bloch states which are periodic and extend across the system. The localised Wannier states are superpositions of Bloch states and are therefore not energy eigenstates. This is what leads to the second term in equation (3.30), which represents tunnelling of atoms between nearest neighbour sites. The tunnelling amplitude, $J$, is proportional to the likelihood of tunnelling between neighbouring sites. The amplitude for tunnelling between sites further apart will be much smaller so only nearest neighbour tunnelling is included. The tunnelling amplitude is calculated from

$$J = -\int d\mathbf{x} w^*(\mathbf{x}) \left( -\frac{\hbar^2}{2M} \nabla^2 + V_L(\mathbf{x}) \right) \left( w(\mathbf{x} - \frac{\lambda L}{2} \hat{x}) - w(\mathbf{x}) \right)$$

where $\hat{x}$ is the unit vector along $x$. When the secondary lattice is included, there will be an additional site-dependent correction to the tunnelling amplitude given by

$$\Delta J_{ij} = -\int d\mathbf{x} w^*(\mathbf{x} - \mathbf{x}_i) V_{\text{dis}}(\mathbf{x}) w(\mathbf{x} - \mathbf{x}_j)$$

This effect of the disorder potential on the tunnelling amplitude is generally small and can be omitted.

The final term in the Bose-Hubbard Hamiltonian is the onsite interaction. This term arises from contact interactions between atoms at the same site. The onsite interaction strength, $U$, is given by

$$U = g \int d\mathbf{x} |w(\mathbf{x})|^4$$

Interactions between atoms at different sites are not included as the contact interaction is local and there is little overlap between atom densities at two different sites. If long-range interactions such as dipolar interactions were to be included, interactions between atoms at different sites may become important.

### 3.2.2 Lattice Equations

The derivation of the HFBP equations for the lattice system proceeds as in the general case outlined in section 3.1, but starting from the Bose Hubbard Hamiltonian. Instead of applying the ansatz (3.7) to the field operator, we apply it to the lattice site creation and destruction operators, that is, we write

$$\hat{a}_i = z_i + \hat{\delta}_i$$

where $z_i$ is a c-number and $\hat{\delta}$ a fluctuation operator. We then follow the steps of section 3.1 to obtain the GPE and BdG equations for the system. Equation (3.37) is
substituted into the Bose Hubbard Hamiltonian and the terms cubic and quadratic in $\delta_i$ are handled with the mean-field approximation. The grand-canonical Hamiltonian, $\hat{K}_{BH} = H_{BH} - \mu$, is minimised to give the generalised GPE,

$$\varepsilon_i z_i - J \sum_{<j>} z_j + U(n_{c_i} + 2\tilde{n}_i) z_i = \mu z_i \tag{3.38}$$

where the sum over $< j >$ is to be taken over the nearest neighbours to site $i$ and the quantities $n_{c_i}$ and $\tilde{n}_i$ are defined by $n_{c_i} = |z_i|^2$ and $\tilde{n}_i = \langle \delta_i^\dagger \delta_i \rangle$.

The BdG equations for the system are given by,

$$\hat{L} u_i^q + \hat{M} v_i^q = E_q u_i^q \tag{3.39}$$

$$\hat{L} v_i^q + \hat{M} u_i^q = E_q v_i^q$$

where $\hat{L} = \hat{h}_o - \mu + Un_{c_i}$, $\hat{M} = -Un_{c_i}$ and $\hat{h}_o$ is the GPE operator defined by $\hat{h}_o z_i = \mu z_i$. The index $i$ continues to label the lattice site while the index $q$ labels the different excitations.

### 3.2.3 Synthetic Magnetic Field

Trapped systems of neutral atoms can provide a well controlled environment to explore the many-body phenomena often associated with solid-state systems. In particular, atoms in optical lattices can be used as a model for crystalline electronic systems. One limitation of this is that the neutral atoms will not respond in the same way to an applied magnetic field. A number of experimental methods have been suggested to replicate the effect of a magnetic field on charged particles for neutral particles trapped in optical lattices [64, 65, 66]. This would allow the exploration of magnetic field field effects in a controlled environment.

We will examine a system with a uniform magnetic field in the direction normal to the plane of the optical lattice. In the tight binding model, the magnetic field enters via phase factors attached to the tunnelling terms in the GPE. These are the Peierls phase factors and they ensure that a particle which traverses a closed path along the lattice gains a phase of $q\Phi/h$, where $q$ is the charge of the particle and $\Phi$ is the magnetic flux through the path. This is consistent with the standard Aharonov-Bohm effect. Boykin et al.[67] have shown that simply by assuming gauge invariance, the addition of phase factors is the full and correct implementation of the magnetic field. Our choice of vector potential determines which tunneling terms have phase factors. In the the Landau gauge, the vector potential is given by $\mathbf{A} = Bx\hat{y}$
and the phase factors are attached to tunnelling in the $y$ direction giving the GPE,

$$
\varepsilon_{jk} z_{jk} - J (z_{j-1,k} + z_{j+1,k} + e^{-i\gamma z_{j,k-1}} + e^{i\gamma z_{j,k+1}}) + U(n_{cjk} + 2\tilde{n}_{jk})z_{jk} = \mu z_{jk}
$$

(3.40)

where

$$
\gamma = q\Phi_0 \hbar
$$

(3.41)

is the phase gained by a particle which moves around one lattice plaquette, and $j$ and $k$ are the lattice indices in the $x$ and $y$ directions respectively. The quantity $\Phi_0$ is the flux through a single lattice plaquette. The proposed methods for producing synthetic magnetic fields for neutral atoms in a lattice essentially work by reproducing the Peierls phase factors.

### 3.3 Dipolar HFBP

Our second application of the HFBP method is to the case of a dipolar BEC. The standard approach to treating interparticle interactions in a BEC is to approximate the interactions as contact interactions [22]. This amounts to using a pseudo-potential of the form $V(x' - x) = g\delta(x' - x)$. The strength of the interaction is characterised by $g$ which is defined in terms of the $s$-wave scattering length, $a_s$, by

$$
g = \frac{4\pi\hbar^2 a_s}{M},
$$

(3.42)

where $M$ is the atomic mass. This is justified by restricting ourselves to dilute gases where the condensate wavefunction varies slowly over the range where there is significant structure in the interaction potential.

This approach is of course invalid if there is long range structure in the interactions. This is clearly the case for dipole-dipole interactions which are both long-range and anisotropic. In our treatment of these interactions we will assume that the dipoles are all aligned by some external field. The dipole moments of each particle are therefore incapable of rotating relative to each other or the trap. In this case the interaction potential is given by [23, 68]

$$
V_{dd}(x) = d^2 \frac{1 - 3\cos^2 \theta}{|x|^3}
$$

(3.43)

where $d$ is the dipole strength, and $\theta$ is the angle between the dipole moment (along the $z$ axis) and the separation vector, $x$.

In general we would like to include both contact and dipolar interactions so our full interaction potential should be $V(x) = g\delta(x' - x) + V_{dd}(x)$. When this is inserted into the generalised GPE (3.21), the contact interactions are easy to handle and we
\[ H_{sp} + gn_c(x) + 2g\tilde{n}(x) + \Phi_D(x) \varphi_0(x) + \Phi_E[x; \varphi_0(x')] = \mu \varphi_0(x) \quad (3.44) \]

where \(n_c(x) \equiv |\Phi(x)|^2\), and \(\Phi_D(x)\) and \(\Phi_E[\varphi_0(x)]\) are the dipolar direct and exchange interactions respectively. The direct interaction is given by

\[
\Phi_D(x) = \int dx' V_{dd}(x' - x) (n_c(x') + \tilde{n}(x')) \quad (3.45)
\]

while the exchange interaction is

\[
\Phi_E[x; \varphi_0(x')] = \int dx' \tilde{n}(x', x) V_{dd}(x' - x) \varphi_0(x') \quad (3.46)
\]

The exchange term involves only the thermal one body density matrix as there is no exchange interaction from the condensate on itself. Note the factor of two in front of the thermal contact interaction term in equation (3.44). This factor arises from the fact that the direct and exchange interactions are identical for contact interactions. The BdG equations for the system are given by equation (3.23).

We will consider a harmonically trapped system with cylindrical symmetry. The external trapping potential for this system is

\[
V_{tr}(x) = \frac{1}{2} (\omega_\rho^2 \rho^2 + \omega_z^2 z^2) \quad (3.47)
\]

where \(\rho\) and \(z\) are the radial and axial coordinates, and \(\omega_\rho\) and \(\omega_z\) are the corresponding trapping frequencies. The dipole moments of the atoms are assumed to be aligned along the \(z\) axis of the trap by an external field.

Both the external and interaction potentials are cylindrically symmetric about the \(z\) axis, so the physically 3D problem can be reduced to a 2D numerical problem. To do this we use the algorithm developed by Ronen et. al. \[28, 30\]. The main difficulty in dealing with dipolar interactions is the divergence and rapid angular variation of the potential at the origin. This makes the evaluation of the integrals (3.45) and (3.46) difficult. Direct numerical integration can be done by introducing a cutoff at small distances to avoid the divergence and integrating on a very fine grid where the integral varies rapidly [68]. This is numerically intensive and care must be taken to ensure the result is independent of the cutoff.

An alternative approach is to perform the integrals in momentum space [27]. Equation (3.45) has the form of a convolution and can be dealt with using the convolution theorem,

\[
\Phi_D(x) = \mathcal{F}^{-1} \left[ \mathcal{F} \left( V_{dd}(k)(n_c(k) + \tilde{n}(k)) \right) \right] \quad (3.48)
\]
where $F^{-1}$ is the inverse Fourier transform, and $\hat{V}_{dd}(\mathbf{k})$, $\hat{n}_c(\mathbf{k})$ and $\hat{n}$ are the Fourier transforms of their position space counterparts.

The dipolar exchange term, (3.46), is not in the form of a convolution due to the non-separable dependence of $\hat{n}(\mathbf{x}', \mathbf{x})$ on its arguments. The integral can, however, still be carried out in momentum space to avoid the divergence. We rewrite the exchange integral as

$$\Phi_E[\mathbf{x}, \varphi_0(\mathbf{x}')] = \frac{1}{(2\pi)^3} \int d\mathbf{k} \mathbf{e}^{i\mathbf{k} \cdot \mathbf{x}} \hat{V}_{dd}(\mathbf{k}) f(\mathbf{x}, \mathbf{k})$$

where

$$f(\mathbf{x}, \mathbf{k}) = \int d\mathbf{x}' e^{-i\mathbf{k} \cdot \mathbf{x}'} \hat{n}(\mathbf{x}', \mathbf{x}) \varphi_0(\mathbf{x}')$$

One important difference between the direct and exchange integrals is that equation (3.48) is a Fourier transform while (3.49) is not, due to the $\mathbf{x}$ dependence of $f(\mathbf{x}, \mathbf{k})$. This means that techniques for evaluating Fourier transforms cannot be applied to equation (3.49).

Using Fourier transforms to perform the integrals in momentum space has the advantage of avoiding the divergence in the dipolar interaction potential, however, in the implementation of [27], using 3D Fourier transforms, the cylindrical symmetry is not taken advantage of. The authors of [28] combine these advantages by using 2D Fourier-Hankel transforms. Because the problem is cylindrically symmetric about the $z$ axis, we assume that the eigenstates of the GPE are eigenstates of $z$ angular momentum so they have the form, $f(\mathbf{x}) = e^{im\varphi} G(\rho, z)$, where $(\rho, \varphi, z)$ are the standard cylindrical coordinates and $m$ is an integer. We can analytically carry out the angular integral of the Fourier transform for such a function,

$$\tilde{f}(k_\rho, k_\varphi, k_z) = \int d\rho \int dz \int d\varphi \rho e^{ik_\varphi \varphi} e^{ik_\rho \rho \cos(\varphi - k_\varphi)} f(\rho, \varphi, z)$$

where $(k_\rho, k_\varphi, k_z)$ are the cylindrical coordinates in momentum space and $J_m(x)$ is the $m$th order Bessel function of the first kind. This leaves a 1D Fourier transform in the $z$ direction and a 1D Hankel transform in the radial direction. We use the following notation for the combined Fourier-Hankel transform of $m$th order,

$$\mathcal{F}{\mathcal{H}}_m[G(\rho, z)] = 2\pi \int dz e^{ik_z z} \int d\rho \rho J_m(k_\rho \rho) G(\rho, z)$$

From equation (3.52) we can see that the full 3D Fourier transform of a function
\( f(x) = e^{i m \phi} G(\rho, z) \) is given by

\[
\tilde{f}(k_\rho, k_\phi, k_z) = i^{-m} e^{ik\phi} \mathcal{F} \mathcal{H}_m[G(\rho, z)]
\]  

(3.54)
Chapter 4

Numerical Methods

The HFBP formalism provides us with a set of coupled non-linear equations for the ground and excited states of the condensate. The Gross-Pitaevskii equation describes the condensate while the Bogoliubov-de Gennes equations describe the excited modes. We must solve these equations self-consistently due to the coupling introduced by the interactions between condensed and non-condensed atoms. The computational method generally follows the following steps:

1. Solve the GPE to obtain the condensate density and chemical potential (ignoring the thermal cloud initially).
2. Solve the BdG equations for the excitations in the presence of a condensate.
3. Populate the excited modes with the Bose distribution to obtain the properties of the thermal cloud.
4. Repeat from step 1, but now include the thermal cloud. Stop when self-consistent.

There are various ways to implement these steps and the two systems we wish to look at require different implementations.

4.1 Dipole Implementation

To solve the dipolar HFBP problem, we use a method based on the work of Ronen et al. [28, 30]. The GPE is solved on a position space grid, using Fourier-Hankel transforms for the kinetic energy and dipolar interaction terms. We find both the ground state (condensate) solution and higher energy solutions of the GPE. We do not attribute any physical significance to the higher energy modes. Instead, they are used as the basis for solving the BdG equations. The properties of the thermal cloud are then calculated and expressed on the position space grid for use in the next iteration of the GPE.
### 4.1.1 2D GP Equation

We use the cylindrical symmetry of the problem to reduce the three-dimensional system to a two-dimensional calculation. Because the solutions of the GPE must be eigenstates of $\hat{L}_z$, they may be assumed to have the form, $\psi(\mathbf{x}) = e^{im\phi}\psi(\rho, z)$. Substituting this into the GPE (3.44) gives

$$
\left[\hat{H}_{sp} + gn_c(\rho, z) + 2\gamma\bar{n}(\rho, z) + \Phi_D(\rho, z)\right]e^{im\phi}\psi(\rho, z) + \Phi_E[\rho, \varphi, z; e^{im\phi}\psi(\rho, z)] = \mu e^{im\phi}\psi(\rho, z). \quad (4.1)
$$

First we’ll look at the single particle Hamiltonian. The trap potential presents no problem on the position space grid, however, calculating the kinetic energy using finite differences would be a poor choice as we will be using a non-uniform grid to maximise the accuracy of our Fourier-Hankel transforms. With this in mind, we will instead apply the Fourier-Hankel transforms to the evaluation of kinetic energy. To do this, apply the Fourier transform and its inverse to the kinetic energy term,

$$
-\frac{\hbar^2}{2M}\nabla^2\psi(\mathbf{x}) = \frac{1}{(2\pi)^3} \int \frac{dk}{\rho} e^{ik\mathbf{x}} \int d\mathbf{x} e^{-ik\mathbf{x}} \left(-\frac{\hbar^2}{2M}\nabla^2\psi(\mathbf{x})\right). \quad (4.2)
$$

The position integral can be done by parts to move the Laplacian to the exponential. This simply gives a factor of $-k^2$ so the kinetic energy can be calculated in the following way

$$
-\frac{\hbar^2}{2M}\nabla^2\psi(\mathbf{x}) = \mathcal{F}^{-1}\left[h^2k^2\frac{1}{2M}\mathcal{F}[\psi(\mathbf{x})]\right]. \quad (4.3)
$$

In terms of Fourier-Hankel transforms for eigenstates of $\hat{L}_z$ we have

$$
-\frac{\hbar^2}{2M}\nabla^2 e^{im\phi}\psi(\rho, z) = e^{im\phi}\mathcal{F}\mathcal{H}^{-1}_m\left[h^2k^2\frac{1}{2M}\mathcal{F}\mathcal{H}_m[\psi(\rho, z)]\right]. \quad (4.4)
$$

We can see from the above equation that when we are looking for a solution with a $z$ angular momentum of $m$, we need to use the $m$th order Hankel transform.

Our main reason for using Fourier transforms in the first place was to tackle the dipolar interaction terms. The direct dipolar interaction has the form of a convolution so it can be written in the form given in equation (3.48). All of the quantities to be Fourier transformed are real and cylindrically symmetric so we can simply replace the 3D Fourier transforms with zeroth order Fourier-Hankel transforms. This leads to the expression

$$
\Phi_D(\rho, z) = \mathcal{F}\mathcal{H}_0^{-1}\left[\tilde{V}_{dd}(k_\rho, k_z)(n_c(k_\rho, k_z) + \bar{n}(k_\rho, k_z))\right], \quad (4.5)
$$
where \( n_c(k_p, k_z) = \mathcal{F} \mathcal{H}_0[n_c(\rho, z)](\tilde{n}(k_p, k_z)) \) (\( \tilde{n}(k_p, k_z) \) similar). The form of \( \tilde{V}_{dd} \), the Fourier transform of the dipolar interaction potential, will be discussed in section 4.1.3.

The exchange dipolar interaction is calculated from equations (3.49) and (3.50). Equation (3.50) is a Fourier transform, however, it cannot be converted into a single Fourier-Hankel transform as \( \tilde{n}(x', x) \) has a non-trivial angular dependence. Physically, this is because \( \tilde{n}(x', x) \) relates to correlations between the points \( x' \) and \( x \). The correlation between two points will, in general, depend on the azimuthal angle between them. The angular dependence can be determined from equation (3.26). We will see in section 4.1.2 that the excitations are also eigenstates of \( \hat{L}_z \) so they can be written in the form

\[
\begin{align*}
  u_i(x) &= e^{i\rho \phi} u_{jm}(\rho, z) \\
  v_i(x) &= e^{i\rho \phi} v_{jm}(\rho, z),
\end{align*}
\]  

(4.6)

where the index \( j \) specifies each of the excitations within a particular \( m \) subspace. We can then use equation (3.26) to write down the thermal density matrix with explicit angular dependence

\[
\tilde{n}(x', x) = \sum_{m'} e^{-im'(\varphi' - \varphi)} \tilde{n}_{m'u}(\rho', \rho, z', z) + e^{im'(\varphi' - \varphi)} \tilde{n}_{m'v}(\rho', \rho, z', z),
\]  

(4.7)

where we have defined

\[
\begin{align*}
  \tilde{n}_{m'u}(\rho', \rho, z', z) &\equiv \sum_j u_{jm'}^*(\rho', z')N_{BE}(E_{jm'})u_{jm}(\rho, z) \\
  \tilde{n}_{m'v}(\rho', \rho, z', z) &\equiv \sum_j v_{jm'}^*(\rho', z')(1 + N_{BE}(E_{jm'}))v_{jm}(\rho, z).
\end{align*}
\]  

(4.8)

We can use equation (4.7) to express the dipolar exchange operator in terms of Fourier-Hankel transforms. The full derivation is given in appendix A. The resulting expression for \( \Phi_E \) is

\[
\Phi_E[\rho, \varphi, z, e^{i\rho \varphi} \psi(\rho', z')] = \frac{e^{i\rho \phi}}{(2\pi)^2} \int dk_p k_p \int dk_z e^{ik_z z} \tilde{V}_{dd}(k_p, k_z) \tilde{f}(\rho, z, k_p, k_z),
\]  

(4.9)

where

\[
\tilde{f}(\rho, z, k_p, k_z) = \mathcal{F} \mathcal{H}_m'[\tilde{n}_{ou}(\rho', \rho, z', z) + \tilde{n}_{ov}(\rho', \rho, z', z)]\psi(\rho', z')J_m(k_p \rho) \\
+ \sum_{m' = 1}^{\infty} \{ \mathcal{F} \mathcal{H}'_{m' - m'}[\tilde{n}_{m'u}(\rho', \rho, z', z) + \tilde{n}_{m'v}(\rho', \rho, z', z)]\psi(\rho', z')J_{m' - m'}(k_p \rho) \\
+ \mathcal{F} \mathcal{H}'_{m' + m}[\tilde{n}_{m'u}(\rho', \rho, z', z) + \tilde{n}_{m'v}(\rho', \rho, z', z)]\psi(\rho', z')J_{m' + m}(k_p \rho) \}. \]  

(4.10)

Evaluating equations (4.9) and (4.10) is the most numerically intensive part of the
calculation. This term has not previously been included in 3D HFBP calculations such as those performed by Ronen and Bohn [30].

We can now eliminate the angular dependence in equation (4.1) leaving us with a two dimensional GPE to solve,

$$\hat{H}_{\text{sp}} + gn_c(\rho, z) + 2gn(\rho, z) + \Phi_D(\rho, z; \psi(\rho, z)) \psi(\rho, z) + \Phi_E(\rho, z; \Psi(\rho, z)) = \mu \psi(\rho, z).$$

(4.11)

In this equation the operators $^H_{\text{sp}}$ and $\Phi_E$ should be thought of as 2D operators. The corresponding 3D operators will simply produce a factor of $e^{im\phi}$ when acting on eigenstates of $\hat{L}_z$ as can be seen in equations (4.4) and (4.9). The meaning of these operators should always be clear from context. To solve (4.11) for eigenstates with different values of $m$, the appropriate Hankel transforms must be used.

### 4.1.2 BdG Equations

Our approach to solving the BdG equations uses the solutions of the GPE, minus the condensate solution, as a basis [61]. This ensures that the excitations we find will be orthogonal to the condensate as we would expect based on the expansion (3.4). If we do not require the excitations to be orthogonal to the condensate, we will find the same energy eigenvalues but, in general, different eigenstates [69].

The BdG equations, (3.23), overdetermine the excitations. We can decouple the equations by defining new amplitudes, $\psi_i^+(x) = u_i(x) + v_i(x)$ and $\psi_i^-(x) = u_i(x) - v_i(x)$ [61]. The decoupled equations for $\psi_i^+$ and $\psi_i^-$ are

$$\hat{h}_0 - \mu + 2\hat{M} \psi_i^+(x) = E_i^2 \psi_i^+(x),$$

(4.12)

$$\hat{h}_0 - \mu + 2\hat{M} \psi_i^-(x) = E_i^2 \psi_i^-(x).$$

(4.13)

These equations are not independent and we will only solve the first. The solutions are related by $(\hat{h}_0 - \mu) \psi_i^+(x) = E_i \psi_i^-(x)$.

To express equation (4.12) with respect to the GPE basis we expand $\psi_i^+(x)$ as $\psi_i^+(x) = \sum_{a=1}^{\infty} c_a^i \varphi_a(x)$, where $\varphi_a(x)$ are the solutions of the GPE. The sum starts from $a = 1$ to exclude the condensate solution, $\varphi_0(x)$. We substitute this expansion into (4.12) and project onto the GPE basis giving

$$\sum_a c_a^i \int dx \varphi_a^*(x) (\hat{h}_0 - \mu + 2\hat{M}) \varphi_a(x) = E_i^2 c_i^a.$$  

(4.14)

which is a matrix eigenvalue equation for the $c_a^i$. Because the $\varphi_a$ obey the GPE
\[ \hat{h}_a \varphi_a(x) = \varepsilon_a \varphi_a(x) \] for eigenvalues \( \varepsilon_a > \mu \), this equation can be simplified to

\[ \sum_a [(\varepsilon_a - \mu) \delta_{ya} + 2M_{ya}] (\varepsilon_a - \mu) c_i^a = E_i^a c_i^a \] (4.15)

where \( M_{ya} = \int dx \varphi_y^*(x) \hat{M} \varphi_a(x) \). To solve this equation we must first evaluate the elements of the matrix \( M_{ya} \). From equation (3.14) the definition of \( \hat{M} \) is \( \hat{M} \psi(x) = \Phi(x) \int dx' \Phi(x') V(x' - x) \psi(x') \). Using this to evaluate \( M_{ya} \) we get

\[ M_{ya} = g \int dx \varphi_y^*(x) n_c(x) \varphi_a(x) + \int dx \varphi_y^*(x) \Phi(x) \int dx' V_{dd}(x' - x) \varphi_a(x') \Phi(x'). \] (4.16)

To avoid the singularity in \( V_{dd}(x' - x) \) we apply the convolution theorem to the \( x' \) integral to convert it to a \( k \)-space integral. This gives

\[ M_{ya} = g \int dx \varphi_y^*(x) n_c(x) \varphi_a(x) + \frac{1}{(2\pi)^3} \int dk \hat{\varphi}_y^*(k) V_{dd}(k) \varphi_a(k) \] (4.17)

where \( \hat{\varphi}_a(k) = \int dx e^{-ik \cdot x} \varphi_a(x) \Phi(x) \).

To perform these integrals on the 2D \((\rho, z)\) grid we use the explicit angular dependence of \( \varphi_a \). The contact interaction term becomes

\[ g \int dx \varphi_y^*(x) n_c(x) \varphi_a(x) = g \int d\varphi \ e^{i(m'-m)\varphi} \int d\rho \rho \int dz \varphi_y^*(\rho, z) n_c(\rho, z) \varphi_{am}(\rho, z) \]

\[ = g \delta_{m'm} \int d\rho \rho \int dz \varphi_y^*(\rho, z) n_c(\rho, z) \varphi_{am}(\rho, z) \] (4.18)

which is clearly diagonal in the quantum number \( m \). One can also show that the same is true for the dipolar interaction term, and consequently the entire matrix \( M_{ya} \). The eigenvalue equation (4.15) is therefore diagonal in \( m \) and can be solved separately in each \( m \) subspace. This implies that the Bogoliubov excitations are also eigenstates of \( \hat{L}_z \).

We can now solve equation (4.15) for \( c_i^a \) which are the coefficients of \( \psi_i^+(x) \) with respect to the GPE basis. Because the \( \psi_i^-(x) \) solutions are simply given by \( \psi_i^-(x) = (\hat{h}_0 - \mu) \psi_i^+(x) / E_i \), we can obtain the \( u_i \) and \( v_i \) from

\[ u_i(x) = \frac{1}{2} \sum_a \left( 1 + \frac{\varepsilon_a - \mu}{E_i} \right) c_i^a \varphi_a(x) \]

\[ v_i(x) = \frac{1}{2} \sum_a \left( 1 - \frac{\varepsilon_a - \mu}{E_i} \right) c_i^a \varphi_a(x). \] (4.20)

There are infinitely many modes to find in principle. In practice we need to limit the number of modes we solve for. To do this we introduce a cutoff energy, \( E_{cut} \), and
find only the modes with an energy lower than this. Once this energy cutoff is introduced, we are limited to temperatures low enough that the highest energy modes calculated are negligibly occupied. Because the numerical difficulty of the problem increases very quickly as the energy cutoff is increased, this places severe restrictions on the temperatures for which we can accurately produce results. One way to overcome this limitation is to use a semiclassical approximation above the cutoff [28, 70]. This approach has not been pursued here as the semiclassical calculations for this system are not trivial to implement.

Once the BdG equations have been solved for the excitation amplitudes, $u_i(x)$ and $v_i(x)$, and energies, $E_i$, we must calculate the thermal one body density matrix and density to use as inputs to the next iteration of the GPE. The contributions to the thermal density matrix from $u_i$ and $v_i$ are given by equation (4.8). These are used to calculate the dipolar exchange term, $\Phi_E$. The thermal density is easily obtained from the contributions to the density matrix by equation (4.7) with $x' = x$ giving

$$\tilde{n}(\rho, z) = \sum_{m'} \tilde{n}_{m'u}(\rho, \rho, z, z) + \tilde{n}_{m'v}(\rho, \rho, z, z).$$ (4.21)

This is used to calculate the contact and direct dipolar interaction terms.

### 4.1.3 Dipolar Interaction Potential

The dipolar interaction potential in position space, $V_{dd}(x)$, is given by equation (3.43), however, the singular behaviour of the potential at the origin makes integrals involving it difficult. To avoid this problem, we use its Fourier transform, $\tilde{V}_{dd}(k)$, which is not divergent. The Fourier transform of the potential is [27]

$$\tilde{V}_{dd}(k) = \frac{4\pi}{3} d^2 \frac{k^2}{k^2} - 1. \tag{4.22}$$

Although this expression is exact, there is subtle problem using it for calculations on a finite grid. For simplicity, imagine we have a cubic position space grid extending from $-R$ to $R$ in each direction. When we take the Fourier transform of quantities, such as the density, on this grid, there is an implicit assumption that the quantity is periodic in each dimension with a period of $2R$. By using the analytical expression (4.22) for the dipolar potential, we allow interactions on any length scale. This dissonance introduces the possibility of interaction between the system and spurious copies located at intervals of $2R$, slowing the increase in accuracy with greater $R$.

One solution to this problem is to cut off the dipolar interaction potential. If we make the potential equal to zero for $r > R$, then we eliminate the possibility of interactions between condensate copies. The Fourier transform of this modified
potential is given by
\[ V_{dd}(k) = \frac{4\pi}{3} \left( 1 + 3 \frac{\cos(Rk)}{R^2 k^2} - 3 \frac{\sin(Rk)}{R^3 k^3} \right) \left( 3 \frac{k^2}{k^2} - 1 \right). \] (4.23)

This form of \( V_{dd}(k) \) is convenient for roughly spherical traps as we can use a grid with similar ranges in \( \rho \) and \( z \) directions. For highly pancake or cigar traps, we generally want to adjust the shape of the grid to match the shape of the trap for maximum efficiency. In this case it would be best to cut the interaction off the same way as the grid, otherwise we will either have the problem of the interaction not covering the extent of the system in the loose direction or there will be interactions between copies in the tight direction. We should therefore make the interaction zero outside a cylinder of radius \( R \) and height \( 2Z \). This leads to a Fourier transformed interaction given by
\[ V_{dd}(k) = \frac{4\pi}{3} \left( 3 \frac{k^2}{k^2} - 1 \right) + 4\pi e^{-Zk} \left[ \sin^2 \alpha \cos(Zk z) - \sin \alpha \cos \alpha \sin(Zk z) \right] \]
\[ - 4\pi \int_R^\infty d\rho \rho \int_0^Z dz \cos(k z) \left( \rho^2 - 2z^2 \right)^{5/2} J_0(k\rho), \] (4.24)
where \( \cos^2 \alpha = k^2 / k^2 \). While this expression is not analytical, and requires an integral to be performed for every grid point, it only needs to be calculated once for a particular grid. This is the form of the dipolar interaction potential used in our calculations.

### 4.1.4 Hankel Transforms

The evaluation of the dipolar interaction terms rely on having an efficient way of performing Hankel transforms. We use the same method as Ronen et al. [28] which was originally derived to apply to cylindrically symmetric optical beams [72]. This method involves sampling the function to be transformed on a non-uniform grid, similar to Gaussian quadrature. To calculate the \( m \)th order Hankel transform of a function \( f(\rho) \), we must sample the function at \( N \) points
\[ \rho_j = \alpha_{mj} / K \] (4.25)
and its Hankel transform at \( N \) points,
\[ k_i = \alpha_{mi} / R \] (4.26)
where \( \alpha_{mj} \) is the \( j \)th root of the Bessel function \( J_m(\rho) \) and \( j \) runs from 1 to \( N \). The values \( K \) and \( R \) are the maximums of the the \( k \) and \( \rho \) grids respectively. Following
Ronen et al. [28], we set $N$ and $R$ and then choose $K = \alpha_{m,N+1}/R$. The $m$th order discrete Hankel transform can then be evaluated from

$$
\tilde{f}(k_i) = \frac{2}{K^2} \sum_{j=1}^{N} \tilde{f}(\rho_j) \frac{J_{m+1}(\alpha_{mj})}{J_m(\alpha_{mi}K)} .
$$

(4.27)

This formula is essentially a matrix multiplication and it allows accurate and efficient calculation of the dipolar interaction terms.

Equation (4.27) allows us to calculate $m$th order discrete Hankel transforms of functions on an $m$th order grid. We often need to perform transforms for functions defined on different grids. This requires us to interpolate functions from one grid onto another. A particularly accurate interpolation method for going between different $m$ grids can be found in reference [73] and in the appendix of reference [28]. This is the interpolation scheme we have used.

We also need to calculate integrals in cylindrical coordinates on our chosen grids, with the general form,

$$
I = \int_0^\infty f(\rho) \rho d\rho
$$

(4.28)

If the function is defined on the $m$th order grid we use the following approximate formula [28],

$$
I = \frac{2}{K^2} \sum_{i=1}^{N} \frac{1}{J_{m+1}(\alpha_{mi})} f(\alpha_{mi}/K).
$$

(4.29)

### 4.2 Lattice Implementation

The solution of the lattice HFBP equations, (3.38) and (3.39), is straightforward compared to the dipolar equations. The GPE is already in the form of a discrete eigenvalue problem and it can be solved by standard matrix diagonalisation techniques. As with the dipolar GPE, we solve for all of the eigenvectors and use these as the basis in which to solve the BdG equations. The BdG equations are again decoupled and solved in the same way as the dipolar BdG equations.

Because we are only considering contact interactions for the bichromatic lattice, the direct and exchange terms for the thermal cloud acting on the condensate are identical and simple to include. There is also no need to introduce an energy cutoff for the calculated modes as there are only a finite number of excited modes equal to the number of lattice sites. For large lattice sizes an energy cutoff can be introduced to speed up calculations, however, we have not done this in the calculations presented here.
Chapter 5

Localisation Results

5.1 Units and Parameters

The main parameters of the problem are the disorder strength, $\Delta$, the strength of interactions, measured by $NU$, where $N$ is the number of particles, and the temperature, $T$. These parameters will all be given in units of the tunnelling energy, $J (J/k_B$ for temperature, where $k_B$ is Boltzmann’s constant). The unit of length is $\lambda L/2$ so that lattice sites are simply labelled by integers, which we call $i$ in the $x$ direction and $j$ in the $y$ direction. We have chosen the ratio, $\lambda L/\lambda_\alpha$ between the primary and secondary lattices, to be the reciprocal of the golden ratio, $(\sqrt{5} - 1)/2$. The offsets for the disorder potential were chosen such that the lattice site with the lowest potential is near the centre of the system. The offsets used were $\delta x = 1.4$ and $\delta y = 5.9$.

5.2 Localisation in 2D

We begin by examining the simplest situation for which localisation can be observed in the 2D disordered lattice. We set the interactions and the temperature to zero. The amount of disorder is then varied by adjusting $\Delta$. Figures 5.1a and 5.1b show the condensate density for $\Delta = 0.43$ and $\Delta = 2.15$ respectively. When there is little disorder, the condensate spreads out across the whole system. Since we are using reflecting boundary conditions, the condensate is non-uniform with its peak density in the centre. If periodic boundary conditions are used, the condensate is uniform when $\Delta = 0$, but as soon as any disorder is introduced, it develops a peak in the centre. This is because the disorder potential necessarily has a different value at opposite ends of the system. For this reason there is little advantage in using periodic boundary conditions.

As the disorder is increased, the condensate becomes concentrated on only a few lattice sites. The signature of Anderson localisation is an exponentially decaying
wavefunction, and hence condensate density. To determine if the condensate is indeed exponentially localised, we plot the logarithm of the condensate density in figures 5.1c and 5.1d. We can see that when there is little disorder, the logarithm is clearly not linear. For $\Delta = 2.15$, there does appear to be a linear decrease from the central peak indicating the localisation of the condensate.

To examine the onset of localisation in more detail, we take a slice of the logarithm along the $x$-axis for the $y$ value where the localised peak occurs. This is plotted in figure 5.2 for various values of $\Delta$. As $\Delta$ is increased, the plots become more linear. It is difficult to determine a precise transition between extended and localised states from these plots. The results suggest that a transition occurs at approximately $\Delta = 2$.

The value for the disorder strength at the transition from extended to localised is the same as that predicted for the Aubry-André model in a one dimensional lattice. This is because the 2-D lattice problem is separable in the absence of interactions.
Figure 5.2: The logarithm of the condensate density for the $j = −3$ cross-section where the localisation is centred. Different curves correspond to different values of $\Delta$ as shown in the legend. Other parameters identical to figure 5.1

The GPE for this case is

$$\varepsilon_{ij}z_{ij} - J(z_{i+1,j} + z_{i-1,j} + z_{i,j+1} + z_{i,j-1}) = \mu z_{ij}. \tag{5.1}$$

Using equation (3.32) we can see that the onsite energy can be split into two terms which are proportional to $\Delta$ and depend on either $j$ or $k$, i.e.

$$\varepsilon_{ij} = \Delta \tilde{\varepsilon}_i + \Delta \tilde{\varepsilon}_j. \tag{5.2}$$

If we look for separable solutions of the form $z_{ij} = X_iY_j$ then we can rearrange equation (5.1) to give

$$\frac{1}{X_i} (\Delta \tilde{\varepsilon}_i X_i - J(X_{i+1} + X_{i-1}) - \mu x X_i) = \frac{1}{Y_j} (\Delta \tilde{\varepsilon}_j Y_j - J(Y_{j+1} + Y_{j-1}) - \mu y Y_j) \tag{5.3}$$

where $\mu_x + \mu_y = \mu$. Both sides of the equation must be equal for all $i$ and $j$ so they must be equal to a constant. This gives the GPE for the 1-D Aubry-Andrè model for both the $x$ and $y$ directions. The value of $\Delta$ at the localisation transition will therefore be the same in the 1-D and 2-D non-interacting cases.
5.3 Interaction Effects

Interactions between particles can complicate the observation of Anderson localisation for the reasons discussed in section 2.2. The interactions can cause self-trapping of the particles or it can break localisation depending on the strength of the interaction and other factors. The presence of self-trapping is strongly dependent on the initial conditions. It relies on the condensate starting in a localised state with a higher energy than the extended ground state. The time-independent HFBP method is not well suited to observing this behaviour as it is concerned with the equilibrium state of a system. We will therefore not explore this behaviour here. Larcher et al. [60] find that, in a one-dimensional incommensurate lattice, self-trapping can be suppressed by using a Gaussian wave packet for the initial condition. It seems reasonable that this result would also hold in a two-dimensional lattice so the effect of self-trapping may be avoided in experiment by preparing the system in a Gaussian shape.

We can try to observe the breaking of localisation by observing whether the exponential character of the wavefunction is destroyed by introducing interactions. In figure 5.3 we have plotted the logarithm of the density for interaction strengths ranging from 0 to $NU = 0.8$ for a disorder strength of $\Delta = 2.15$ where the non-interacting condensate is localised. The linear shape of the logarithm appears to
be broken for $NU = 0.2$ indicating the breaking of localisation. The condensate then spreads out slightly as the interaction strength is increased further. This is consistent with the 1-D results of Larcher et al. [60], who find that, for disorder strengths slightly above the non-interacting transition value, localisation is broken by relatively small interaction strengths. They also find that for increasing disorder strengths, the delocalisation can be suppressed for increasing lengths of time. It is difficult to find a self-consistent solution to the HFBP equations for large disorder strengths and significant interactions, and in any case, it is unlikely we would be able to observe this suppression as it does not appear to persist indefinitely and we can only observe equilibrium properties.

To compare these results with the 1-D lattice experiment of Roati et al. [16], we note that they tune the interaction strength using a Feshbach resonance so that $U \approx 10^{-5}$ (in units of $J$). They also prepare the condensate with approximately $10^5$ atoms. This would imply a value for $NU$ of order 1 which is strong enough to have an effect on the localisation. This may be why the transition from extended to localised states appears to occur for values of $\Delta$ greater than 2. It must also be noted that the given condensate number of $10^5$ applies to the condensate before the magnetic field is changed to reduce the interaction strength. It is not clear if many atoms are lost during this phase which may reduce the interaction energy further.

The introduction of interactions also causes some of the atoms to be pushed out of the condensate. These non-condensate atoms are known as the quantum depletion. In the HFBP formalism they arise from the term in equation (3.26) which does not involve the Bose distribution. It is therefore present at zero temperature and given by

$$n_{\text{dep}} = \sum_q |u_q|^2.$$  \hspace{1cm} (5.4)

For the parameters used in figure 5.3, the quantum depletion always contains less than one atom and consequently has very little effect on the results. The quantum depletion does not display any localisation.

## 5.4 Finite Temperature Effects

We will now examine the effect of temperature on the localisation. To do this we fix the number of condensate atoms at $10^4$ and populate the Bogoliubov modes according to the chosen temperature. The HFBP equations are solved self-consistently and the total number of atoms is given by the sum of the condensate and non-condensate atoms. We use a very small interaction strength of $NU = 10^{-2}$ so that the localisation at zero temperature is not broken by interactions.

We find that the temperature has very little effect on the localisation. To mea-
Figure 5.4: Localisation length and condensate fraction as a function of temperature. The different lines represent different disorder strengths: $\Delta = 2.15$ (blue), $\Delta = 4.30$ (green) and $\Delta = 7.50$ (red). The interaction strength is $NU = 10^{-2}$, there are $10^4$ condensate atoms and the temperature is in units of $J/k_B$. The localisation length is in units of the lattice constant. Since the number of atoms in the condensate is fixed, the total atom number varies with temperature.

The reason the thermal atoms have so little effect on the condensate, even when there are a significant number of them, is that they are spatially separated from it. The condensate occupies the lowest energy mode of the system which is localised about a lattice site. The thermal atoms occupy modes which are spread over the rest of the lattice sites. Since we are only considering contact interactions, and there are very few thermal atoms occupying the same sites as the condensate, the thermal atoms cannot have much effect on the condensate.

The thermal atoms are spread out over many lattice sites and display no ev-
idence of localisation. This is to be expected as Anderson localisation is a wave phenomenon and it should therefore only occur for the coherent part of the system which is the condensate. In an experiment, we would expect the thermal cloud to expand while the condensate remains localised. To observe this numerically would require difficult time-dependent finite temperature calculations.

5.5 Synthetic Magnetic Field

To examine the effect of a synthetic magnetic field on the lattice system, we will solve the HFBP equations using equation (3.40), the generalised GPE with Peierls phase factors. The strength of the magnetic field is controlled by the parameter $\gamma$ which is defined in equation (3.41). The condensate we calculate will now have a non-uniform phase. We can interpret this non-uniform phase as representing particle flow analogous to the superfluid flow in a continuous system. We will associate the particle flow with the probability current density defined by

$$j(x) = \Re \left[ \psi^*(x) \frac{p}{M} \psi(x) \right],$$

where $\psi(x)$ is the wavefunction and $p$ the momentum operator. In the presence of an electromagnetic field, the momentum operator is given by $p = -i\hbar \nabla - qA(x)$ where $q$ is the charge of a particle and $A(x)$ is the vector potential. This leads to the following form for the probability current density,

$$j(x) = \frac{|\psi(x)|^2}{M} (\hbar \nabla \theta(x) - qA(x)),$$

where $\theta(x)$ is the phase of the wavefunction. In the absence of an electromagnetic field ($A = 0$), this leads to the usual association of superfluid velocity with the gradient of the phase. This equation is strictly only true for a continuous system, however, we will interpret this as a coarse-grained flow for the lattice system with the gradients calculated by finite differences.

To begin with, we look at the effect of the field on the translationally invariant lattice, i.e. with disorder turned off. In figure 5.5 we show the condensate density and probability density current for a relatively small synthetic field. The density is basically unchanged from the case with no magnetic field, however, there is now a rotation of the whole system about the centre. This corresponds to the orbits of charged particles in a magnetic field. At larger values of $\gamma$, where a particle gains a significant phase by moving around a single lattice plaquette, we are unable to find an acceptable ground state.

The fact that there appears to be a bulk rotation of the condensate when we ap-
Figure 5.5: Condensate density in a translationally invariant lattice with an applied synthetic magnetic field. The parameters used are $\gamma = 0.01$, $\Delta = 0$, $NU = 0.01$, $T = 2$, and $N = 10^4$. The colour of the surface represents the phase of the wavefunction and the arrows show the direction and relative magnitude of the probability current density.

The synthetic field is very unusual as it is usually the case that superfluid flow is irrotational unless there are vortices present. Here we will show why this bulk rotation can be present in our calculations. We can interpret the probability current density, multiplied by the number of atoms in the condensate, as the condensate density multiplied by its velocity. This gives an expression for the velocity field,

$$v(x) = \frac{1}{M} \left( \hbar \nabla \theta(x) - qA(x) \right).$$  

(5.8)

When there is no synthetic electromagnetic field this velocity field is irrotational as it is simply given by the gradient of the phase. This leads to the usual statement that superfluid flow is irrotational. Rotation can only be present when the phase is discontinuous which implies the presence of vortices. When there is a synthetic field, the curl of the velocity is given by,

$$\nabla \times v = -\frac{qB}{M},$$  

(5.9)

where $B = \nabla \times A$ is the synthetic magnetic field. This implies that the flow of the condensate in a synthetic magnetic field is not irrotational.

The single valued nature of the wavefunction no longer enforces irrotational flow in the condensate, but it will still impose some condition on the flow. To see what
Figure 5.6: Condensate density and probability current density for a disordered system with an applied synthetic magnetic field. Parameters are $\gamma = 0.01$, $\Delta = 2.15$, $NU = 0.01$, $T = 2$, and $N = 10^4$. In figure (a) the colour represents the wavefunction phase.

this condition is, we take the integral of (5.7) around a closed loop and, for a simple case, we take a cylindrically symmetric potential and a circular integration path of radius, $r$, centred on axis of symmetry. The condensate density will be constant along this path so we get,

$$\oint r j \cdot dl = \frac{h}{M} |\psi(r)|^2 \oint r \nabla \theta \cdot dl - \frac{q}{M} |\psi(r)|^2 \oint r A \cdot dl. \quad (5.10)$$

The first integral on the right hand side is just the change in the the phase around the loop. Because the wavefunction must be single-valued, this must be an integer multiple of $2\pi$. By Stokes’ theorem, the second integral on the right gives the ‘magnetic’ flux, $\Phi$, through the loop. We can therefore rewrite equation (5.10) as,

$$\Phi(r) + \frac{M}{q |\psi(r)|^2} \oint r j \cdot dl = \frac{2\pi h}{q} \eta, \quad (5.11)$$

where $\eta$ is an integer. In a superconductor, this equation leads to flux quantisation as the London equation implies that no significant current can flow in the interior of the material. In this case it is a combination of flux and net flow around the loop which is quantised.

To look at what happens for a disordered system, we use the same parameters, but with the disorder strength set to $\Delta = 2.15$. As in the case with no disorder, the condensate density is almost unaffected by the magnetic field. We again get rotation of the condensate and this time the rotation is centred on the localised peak. Using higher magnetic field strengths again leads to unacceptable ground states. For the values of the magnetic field we are able to use, there is no evidence of significant
effect on the localisation of the condensate. It is likely that higher magnetic field strengths will have more effect, but the current method seems to be unsuitable for strong magnetic fields.
Chapter 6

Dipolar BEC Results

6.1 Units and Parameters

A number of schemes for choosing dimensionless parameters have been used in the literature. The energy and length units are usually chosen based on the harmonic trap frequency. In general, the energy unit will be $E_0 = \hbar \omega_{\text{trap}}$ and the length unit, $a_{\text{ho}} = \sqrt{\hbar/M \omega_{\text{trap}}}$. Because the trap is cylindrically symmetric, there are two characteristic frequencies, $\omega_\rho$ and $\omega_z$. We therefore have some choice as to what $\omega_{\text{trap}}$ should be. Ronen et al. [28] use the transverse trapping frequency, $\omega_\rho$. The arithmetic mean of the squares, $\omega_a^2 = \frac{1}{2}(2\omega_\rho^2 + \omega_z^2)$ has been used by Hutchinson and Zaremba [74] in a study of the excitations of a contact gas. Finally, we can also use the geometric mean frequency, $\omega_g = \sqrt[3]{\omega_\rho \omega_z}$. We have used each of these conventions where they are useful and appropriate for comparison with previous work.

To characterise the strength of the dipolar and contact interactions we define the dimensionless parameters,

$$D = N \frac{Md^2}{\hbar^2 a_{\text{ho}}} \quad (6.1)$$

and

$$\tilde{g} = Ng \frac{M}{\hbar^2 a_{\text{ho}}} = 4\pi Na/a_{\text{ho}} \quad (6.2)$$

where $N$ is the number of particles and $a$ is the scattering length. For the finite temperature calculations, we must choose an energy cutoff for the calculation of excited modes. We have used a cutoff of $E_{\text{cut}} = 6\hbar \omega_\rho$ throughout this work. For temperatures $T = \hbar \omega_\rho / k_B$ and below, this cutoff is high enough that the results are reasonably independent of the cutoff.
Figure 6.1: Contour plots of condensate density for contact interactions only (blue) and contact and dipole interactions (green). The density decreases monotonically from the origin. The parameters used are \( \lambda = 1 \) (spherical trap), \( T = \hbar \omega / k_B \), \( \tilde{g} = 1 \), \( N = 10^4 \) and \( D = 3 \) for the dipolar case. The length unit is \( \sqrt{\hbar/M \omega} \).

### 6.2 Density Profiles

Let us examine the solutions of the HFBP equations without including thermal dipolar exchange. The first quantity we will look at is the condensate density. The presence of dipolar interactions alters the shape of the condensate as was seen in the earliest studies of dipolar condensates [23, 24]. The same behaviour occurs at finite temperature as we can see in figure 6.1. When there are only contact interactions present, a condensate in a spherical trap is also spherical. When there are dipolar interactions present, however, the condensate elongates in the axial direction.

This behaviour can be explained by considering the anisotropy of the dipolar potential. Dipoles experience an attractive force when they are aligned head-to-tail rather than side-by-side. A density profile which is elongated along the axial direction, so that more dipoles are aligned head-to-tail, will have a lower energy than one in which the dipoles experience more repulsive forces. This is not a particularly intuitive result as one might expect that the repulsive interactions in the \( x-y \) plane would cause the condensate to expand radially. Since the dipoles are attractive along the axial direction however, they may have a lower energy overall by aligning head-to-tail than they would by simply moving apart. The same behaviour was found at zero temperature by Yi and You [23] for a slightly pancake trap.

The effect of the dipolar interactions on the shape of the condensate is highly dependent on the aspect ratio of the trap [24]. In figure 6.2 we have plotted the
condensate density contours for a cigar trap with $\lambda = 1/7$ and a pancake trap with $\lambda = 7$. In the cigar-shaped trap, the condensate will be elongated in the axial direction. This means that the attractive part of the dipolar interaction will be dominant. In figure 6.2a we can see that the dipolar condensate drops off more steeply from the centre than the contact-only condensate. It also has a higher peak density. The attractive part of the dipolar interaction is ‘pulling’ the condensate in on itself. In this case the dipolar interactions have little effect on the aspect ratio of the condensate.

In the pancake-shaped trap in figure 6.2b we can see that the dipolar interaction affects both the drop-off in density and its aspect ratio. The condensate expands radially with the dipolar interactions and its density decreases more slowly from the centre than the contact-only condensate. This time the dipolar condensate has a lower peak density than the contact-only condensate. In the pancake trap, the repulsive part of the dipolar interaction is dominant and this explains these effects. Unlike in the spherically trapped situation, the condensate does expand radially due to the repulsion of side-by-side dipoles. In this case, the dipoles face a large energy cost for lining up head-to-tail due to the strong axial trapping. The lowest energy state is therefore when the dipoles spread out radially where there is only weak trapping.

We can also look at the non-condensate density. This is given by setting $x' = x$
in equation (3.26) giving,
\[
\hat{n}(x) = \sum_i \{ |u_i(x)|^2 + |v_i(x)|^2 \} N_{BE}(E_i) + |v_i(x)|^2 \}.
\] (6.3)

At zero temperature, \( N_{BE}(E_i) = 0 \) for all \( i \) so the only contribution to the non-condensate density is the quantum depletion, \( \hat{n}(x) = \sum_i |v_i(x)|^2 \). This term generally requires the calculation of very many modes to converge, however, it is usually very small, and at finite temperature it is overwhelmed by the thermal population of the excited modes. The thermal part of the non-condensate converges more quickly as the Bose distribution factor, (3.25), decays exponentially with the mode energy once \( \beta E_i \gg 1 \). The fact that the quantum depletion may not be well converged is therefore not very important once there is an appreciable amount of thermal atoms.

Two examples of non-condensate densities are shown in figure 6.3. The temperature used for these calculations is \( T = \hbar \omega / k_B \). This temperature is high enough that the contribution to the non-condensate density from thermal particles is much greater than that from the quantum depletion. It is also low enough that the energy cutoff of \( E_{\text{cut}} = 6\hbar \omega \rho \) does not significantly affect the result. Figure 6.3a shows the non-condensate density when there are only contact interactions present. The density is spherically symmetric, increasing from the centre of the trap to a maximum at \( \rho^2 + z^2 \approx 1 \) and decreasing thereafter. This ring shaped thermal cloud also occurs when no interactions at all are included. This is simply due to the fact that the lowest modes above the condensate mode have peaks away from the centre of the trap. This ring shaped cloud is enhanced by the presence of contact interactions as the thermal cloud experiences a potential of \( 2gn_c(x) \) from the condensate which pushes it out. Figure 6.3b shows the non-condensate density with dipolar interactions included. Compared with the non-dipolar case, the density is reduced in the \( z = 0 \) plane of the trap and there are two separate peaks at \( z \approx \pm 1 \). The two peaks arise due to the anisotropic dipolar interaction splitting up the ring from the contact interaction case.

### 6.3 Effective Dipolar Potential

If thermal dipolar exchange is being ignored then the effect of dipolar interactions can be thought of as producing an effective potential. The GPE in this case is
\[
\hat{H}_\text{sp} + gn_c(\rho, z) + 2g\hat{n}(\rho, z) + \Phi_D(\rho, z) \psi(\rho, z) = \mu \psi(\rho, z).
\] (6.4)

From the form of the equation we can see that \( \Phi_D(\rho, z) \) simply acts like a potential, just as the contact interaction terms do. A typical example of the shape of this
Figure 6.3: Non-condensate density with (b) and without (a) dipolar interactions. Dark red is the highest density and dark blue is the lowest density. Parameters used are the same as for figure 6.1. Some of the contours are jagged due to the limited spatial resolution. The length unit is $\sqrt{\hbar/M\omega_r}$.

Effective potential is shown in figure 6.4. In the $z = 0$ plane of the system, the effective potential increases with increasing radial distance for $\rho < 1.5$. This is the region in which the condensate has an appreciable density and the potential gradient is consistent with the observation that the condensate is compressed in the radial direction. The bump in the potential along $z = 0$ also explains the reduction in density of the non-condensate here. This effective potential includes the effects from both the condensed and non-condensed particles, however, at the given temperature, the size of the effective potential due to the non-condensed particles is approximately four orders of magnitude smaller.

6.4 Excitations

We will now look at the excitation spectrum of the dipolar BEC. This is the set of eigenvalues, $E_j$, obtained from the Bogoliubov-de Gennes equations (3.23). Previously, the zero temperature Bogoliubov excitations have been studied by Ronen, Bortolotti and Bohn [28]. Ronen and Bohn also looked at the finite temperature excitations without including thermal exchange [30]. They found that the excitation energies are not significantly affected by temperature except near the critical temperature or for highly non-spherical traps (e.g. $\lambda = 7$). The temperatures we can accurately model are limited by the cutoff in energy we use for the Bogoliubov energies. Over this range of temperatures we also find very little change in excitation energies. We will therefore examine the zero-temperature spectrum as it is significantly easier to calculate and displays all of the same features as the small but finite temperature spectrum. We will also ignore the quantum depletion as its effect
is very small and requires many modes to calculate accurately.

First we examine how the excitations are affected by the aspect ratio of the trap. In order to concisely show the full range of trap aspect ratios, we follow the conventions used by Hutchinson and Zaremba [74]. The aspect ratio is characterised by the parameter,

\[ \beta = \frac{2\omega_z^2 - 2(\omega^2_p)^2}{2\omega^2_p + \omega^2_z} \]  

(6.5)

and energy and length scales are defined by the arithmetic mean as defined in section 6.1. The aspect ratio, \( \lambda \), is related to \( \beta \) by

\[ \lambda = \frac{2\beta + 2}{2 - \beta} \]  

(6.6)

The parameter \( \beta \) can range from \(-1\), corresponding to a one-dimensional cigar trap, to \(2\), corresponding to a two-dimensional pancake trap. The trap is spherical when \( \beta = 0 \). Because the trap potential is symmetric on reflection in the \( z = 0 \) plane, the excitations can be split into those with even or odd amplitudes. The excitation energies are plotted against \( \beta \) in figure 6.5.

The lowest \( m = 1 \) even excitation and lowest \( m = 0 \) odd excitation represent the centre of mass or Kohn modes in the radial and axial directions respectively. The Kohn modes should oscillate at the trap frequencies, \( \omega_p \) for the radial mode and \( \omega_z \) for the axial mode, regardless of the interactions present. Their corresponding energies, in units of the mean trap energy, should therefore be given by

\[ \frac{\omega_p}{\omega_a} = \sqrt{1 - \beta/2} \] and \[ \frac{\omega_z}{\omega_a} = \sqrt{1 + \beta} \] for the radial and axial modes respec-
Figure 6.5: Zero temperature excitation energies for a dipolar BEC with $D = 3$ and $\tilde{g} = 1$ ((a) and (b)) and for a non-interacting BEC ((c) and (d)). Different $m$ states are represented by blue circles ($m = 0$), green squares ($m = 1$), red triangles ($m = 2$), cyan crosses ($m = 3$), and pink dots ($m = 4$). The solid black lines show the analytical values for the Kohn modes. Energy and length units are $\hbar \omega a$ and $\sqrt{\hbar/M \omega a}$ respectively.
tively. These analytical expressions have been plotted along with the calculated excitation energies in figure 6.5. There is excellent agreement between the analytical and numerical results indicating no problems with the model or numerics.

The excitation energies for a non-interacting BEC are also plotted in figure 6.5 for comparison with the interacting case. The non-interacting excitations are simply calculated by setting both $D$ and $\tilde{g}$ to zero. The contact interaction used in the dipolar calculation is relatively small and the excitations produced using only this interaction are only slightly different to the non-interacting case. The differences between the dipolar calculation and the non-interacting case are therefore primarily due to the dipole interaction.

The dipolar interaction breaks the degeneracy between various modes. This happens in two ways. Excitation energies corresponding to different values of $m$ are split over a large range of the trap aspect ratio. Higher $m$ excitations are pushed up relative to lower $m$ excitations. For example, the lowest even $m = 2$ excitation is always degenerate with one of the even $m = 0$ excitations in the non-interacting case. When dipolar interactions are included, the $m = 2$ excitation has a higher energy for most aspect ratios. As $\beta$ approaches 2, and the trap becomes more pancake shaped, this energy splitting is reduced. This pattern breaks down for highly pancake traps both when the dipolar interaction is very strong [29] and high temperatures [30].

The dipolar interactions also break the degeneracy of modes of the same angular momentum at the aspect ratios where they would have crossed each other in the non-interacting case. This leads to avoided crossings between excitations of the same angular momentum. The energy differences are quite small making it difficult to see these avoided crossings in figure 6.5. In figure 6.6 the energy splitting

Figure 6.6: Excitation energies at zero temperature in a spherical trap for a range of dipole strengths, $D$. Contact interactions are set to zero so that various modes are degenerate at $D = 0$. 
between modes with the same $m$ value can be seen more clearly for the spherical case. For example the two lowest $m = 0$ even parity modes are degenerate for $D = 0$, but as $D$ increases, one mode decreases in energy while the other increases. In fact, the lower mode goes to zero for slightly larger $D$ indicating the collapse of the condensate.

Contact interactions also break the degeneracy of various modes, but not as completely as dipolar interactions. For the spherical case shown in figure 6.6, a number of modes remain degenerate when only contact interactions are present. For example, take the three modes which are of even parity and degenerate with an energy of $2\hbar\omega$ when no interactions are present. When contact interactions are included, the $m = 2$ mode remains degenerate with one of the $m = 0$ modes, although both shift in frequency. The degeneracy between these two modes and the other $m = 0$ mode is broken. The same pattern holds for the lowest odd parity $m = 2$ mode and the two accompanying $m = 0$ modes, and again for the lowest even parity $m = 3$ mode and the accompanying $m = 1$ modes. Similar patterns hold for higher energy modes. Dipolar interactions break these degeneracies which remain in the contact interaction case.
Chapter 7

Thermal Dipolar Exchange

Ideally, we would like to be able to solve the HFBP equations (4.11) and (4.12) together, self-consistently. This proves to be a very difficult numerical task however. The thermal dipolar exchange term (4.9) is the main problem. Let the number of grid points in the $\rho$ and $z$ directions be approximately $P$, and the total number of $m$ subspaces used be $Q$. The exchange term must be evaluated at each of the $P^2$ grid points. The integral at each point requires the evaluation of the integrand at the $P^2$ grid points. Each evaluation of the integrand requires $2Q$ Fourier-Hankel transforms, and the slowest part of the transform is a $P \times P$ matrix multiplication which scales as $O(P^3)$. A single evaluation of the exchange term therefore scales as $O(QP^7)$. This term must be evaluated many times to find the eigenvalues and eigenvectors of the GPE, and this in turn must be performed a number of times to achieve self consistency.

Because of the above considerations, we have minimised the number of times we need to calculate the thermal exchange term. To do this we calculate the self-consistent solution of the equations without the thermal dipolar exchange term. We then perform a few iterations of the full equation with thermal exchange, using this solution as an initial guess. By doing this we treat the effects of thermal dipolar exchange as a small perturbation. We can then determine the effect it has on properties such as the energy and shape of the condensate, and the energies of the excited modes.

7.1 Calculating the thermal exchange term

Our aim is to evaluate equations (4.9),

$$\Phi_E[\rho, \varphi, z; e^{im\varphi} \psi(\rho', z')] = \frac{e^{im\varphi}}{(2\pi)^2} \int dk_\rho k_\rho \int dk_z e^{ik_z z} V_{dd}(k_\rho, k_z) \tilde{f}(\rho, z, k_\rho, k_z),$$
Figure 7.1: The dipolar exchange term acting on the condensate wave function for parameters, \( D = 1, \tilde{g} = 0.01, \lambda = \sqrt{8}, N = 1000 \) and \( T = 2\hbar \omega_\rho \). The length unit is \( \sqrt{\hbar/M\omega_\rho} \).

We see that in the second equation we must evaluate Fourier-Hankel transforms of various orders for a given thermal density matrix and function \( \psi(\rho, z) \). The Hankel transforms are carried out by using equation (4.27). To calculate the eigenstates of the GPE in a particular \( m \) subspace, the contributions to the thermal density matrix and the trial function, \( \psi(\rho, z) \), must be interpolated onto each of the \( |m' - m| \) and \( m' + m \) grids. The contributions to the thermal density matrix can be interpolated before the calculation of the eigenstates to save time, however, the interpolation of \( \psi(\rho, z) \) must be performed during this calculation. The integration over \( k_z \) in the first equation is done using the basic rectangle method, while the integral over \( k_\rho \) uses the method given in section 4.1.4.

To determine the size of the effect of the thermal exchange term we can examine the quantity \( \Phi_E[x; \varphi_0(x')] \). This gives the interaction of the non-condensate on the condensate via exchange. We cannot define an effective potential for the exchange as we did with the direct dipolar interaction (plotted in figure 6.4). An example of
to the chemical potential from the direct thermal dipolar interaction (green line) and the exchange thermal dipolar interaction (blue line).

Figure 7.2: Effect of the thermal exchange interaction on the chemical potential for $D = 1, \tilde{g} = 0.01, \lambda = \sqrt{8}, N = 1000$ and $T = 2\hbar\omega_\rho$. Plotted for four self-consistency iterations with thermal exchange included. Energy and length units are $\hbar\omega_\rho$ and $\sqrt{\hbar/M\omega_\rho}$ respectively.

The function $\Phi_E[x; \varphi_0(x')]$ is plotted in figure 7.1.

To obtain a convenient measure of the importance of the thermal exchange term, we can look at its contribution to the chemical potential [75]. The chemical potential can be obtained from the GPE by taking the inner product with $\varphi_0(x)$ giving

$$\mu = \int \varphi_0^*(x)\hat{H}_{sp}\varphi_0(x) + (g n_c(x) + 2g\tilde{n}(x) + \Phi_D(x))|\varphi_0(x)|^2 + \varphi_0^*(x)\Phi_E[x; \varphi_0(x')]|d x.$$  \hfill (7.1)

The contribution of thermal exchange is therefore given by

$$\mu_E = \int \varphi_0(x)\Phi_E[x; \varphi_0(x')]|d x.$$  \hfill (7.2)

To determine the importance of this term we can compare it with the contribution from the direct dipolar interaction from the non-condensate. This is given by

$$\mu_D = \int |\varphi_0(x)|^2 \int V_{dd}(x' - x)\tilde{n}(x').$$  \hfill (7.3)

We do not compare with the full direct dipolar interaction as this will be dominated by condensate-condensate interaction at low temperatures.

After calculating the self consistent solution without thermal exchange, we can ‘turn on’ thermal exchange for a few iterations and examine the chemical potential. Figure 7.2 shows an example of this for a pancake trap with $\lambda = \sqrt{8}$ at a temperature $T = 2\hbar\omega_\rho$. Once the thermal exchange is turned on, we can start to calculate its
contribution to the chemical potential from equation (7.2). In figure 7.2a we can see that this contribution is about a fifth of the size of the contribution from the direct thermal interaction. It also lowers the chemical potential, whereas the direct term raises it. Figure 7.2b shows the behaviour of the full chemical potential over the same iterations. It is reduced by an amount consistent with the contribution from the thermal exchange. From these figures we can see that the effect from thermal exchange is small relative to the effect from direct thermal interactions. At this low temperature its absolute effect is also small, and there is little change after the first iteration with thermal exchange included. This suggests that we can get a good idea of the size of the effect by performing only one iteration with thermal exchange.

We have explored the effect of the thermal exchange interaction at a range of temperatures. The cutoff in energy for which we calculate the Bogoliubov modes limits the temperatures we can accurately produce results for. If we ignore this restriction however, we can still estimate the exchange interaction effects from the low energy modes. While this will not produce accurate results for physical quantities, it will allow us to compare the effects from the direct and exchange terms over a greater range of temperatures. In figure 7.3 we have plotted the chemical potential contribution from the thermal direct and exchange terms for temperatures ranging from $5\hbar\omega_\rho$ to $40\hbar\omega_\rho$. We can see that as before the direct effect is positive while the exchange effect is negative and the direct effect is about five times the size of the
Figure 7.4: Excitation energies for the first five iterations with thermal dipolar exchange. Parameters used are $T = 5\hbar\omega_\rho$, $\lambda = \sqrt{8}$, $D = 3.5$ and $\tilde{g} = 0$. The different coloured lines represent the different $m$ modes, $m = 0$ (blue), $m = 1$ (green), $m = 2$ (red), $m = 3$ (cyan) and $m = 4$ (magenta). Energy and length units are $\hbar\omega_\rho$ and $\sqrt{\hbar/M\omega_\rho}$ respectively.

### 7.2 Excitations

In the previous section the size of the thermal dipolar exchange effect was very small. To investigate the effect on the excitation spectrum, we will choose parameters such that the effect is relatively large. In order for the thermal exchange effect to be large, the number of thermal atoms should be a significant fraction of the total number of atoms. For a realistic number of atoms, this would require temperatures much higher than we can accurately handle. We have therefore opted to use a very small condensate of only 100 atoms. We still must have temperatures on the order of the cutoff in energy to produce a significant fraction of thermal atoms which means that we are ignoring modes which would have significant occupation. We used a temperature $T = 5\hbar\omega_\rho$ with an energy cutoff of $6\hbar\omega_\rho$. The other parameters are $\lambda = \sqrt{8}$, $D = 3.5$ and $\tilde{g} = 0$.

The chemical potential for this system without thermal dipolar exchange was found to be $\mu = 2.81\hbar\omega_\rho$ by self-consistent calculation. After 13 iterations with thermal dipolar exchange, the chemical potential has shifted to $\mu = 2.73\hbar\omega_\rho$. This shift is much larger than those calculated in the previous section. In fact, the shift
due to thermal dipolar exchange is almost the same in absolute value as the thermal dipolar direct term in this case. It is still negative while the direct shift is still positive. It may be however, that including higher energy modes would increase the direct effect more than the exchange effect. This is because the direct dipolar effect depends on the condensate density which will certainly increase with the inclusion of more modes. The exchange effect depends on integral of the products of different modes with the dipolar potential. For highly oscillatory, higher energy modes, this integral may become small.

We have plotted the excitation energies for the system up to $E = 5\hbar \omega_p$ in figure 7.4. The energies are plotted for the first few iterations including thermal dipolar exchange. The energies appear to be quite well converged after only a few iterations. All of the excitation energies are shifted up when thermal exchange is included, with the lowest $m = 0$ mode showing the largest increase. The two Kohn modes are also shifted up which is physically incorrect, however this is likely to be due to the limitations of HFBP theory and the shift away from the expected values also occurs when thermal exchange is ignored [30].
Chapter 8

Conclusions

In this work we have applied the HFB-Popov formalism to two problems of current interest: Anderson localisation in a two-dimensional bichromatic lattice and Bose-Einstein condensates with dipolar interactions. By solving the HFBP equations we can determine both the condensate properties and excitation spectrum at finite temperature. For the 2-D bichromatic lattice, we have determined that Anderson localisation occurs for sufficiently strong disorder. We have also examined the effect of contact interactions, finite temperature and synthetic magnetic fields on this localisation. For the dipolar BEC we have explored the effect of the dipolar interactions at finite temperature. We have determined the effect of thermal dipolar exchange interactions by performing the necessary computationally expensive calculations.

8.1 Anderson Localisation

We have shown that Anderson localisation occurs for a non-interacting BEC in a 2-D bichromatic lattice for a disorder strength of about $\Delta = 2J$. This is the same value as for the 1-D bichromatic lattice and this is the expected result as the non-interacting 2-D problem can be separated into two 1-D problems. We then introduce contact interactions between particles and find that they can break the exponential character of the wavefunction, implying the destruction of localisation. We were unable to investigate the phenomenon of self-trapping due to interaction. This requires the condensate to be in an initial state with a high interaction energy. Because we are finding the ground state of the GPE, we cannot examine these states. A time-dependent GPE approach could be used to study self-trapping in the 2-D lattice.

The HFBP method allows us to calculate the effects of finite temperature on the system. For contact interactions, this occurs via an effective potential produced by the particles in thermally occupied states. We find that this thermal cloud has
essentially no effect on the localisation of the condensate even when approximately 25% of the particles are in the thermal cloud. This is because the vast majority of thermal atoms are spatially separated from the localised condensate. The particles can only interact via the short range contact interaction if they are at the same lattice site, so the thermal atoms have little interaction with the condensate. It would be interesting to consider whether thermal atoms with long-range interaction, such as dipole interactions, would break the localisation of the condensate.

By using a two-dimensional bichromatic lattice we can explore the effects of an applied synthetic magnetic field. The synthetic magnetic field reproduces the effect of a magnetic field on charged atoms. In the tight-binding model this leads to Peierls phase factors being attached to the tunnelling terms. The synthetic field causes the condensate wavefunction to acquire a non-uniform phase. By calculating the probability current density, we find that the condensate rotates in the presence of the field. We are unable to calculate a solution for large synthetic fields and it is likely that a time-dependent approach would be better suited to determining the effect of the field on localisation.

8.2 Dipolar BEC

We have examined the effect of dipolar interactions on a harmonically trapped BEC. To begin with, we ignore the thermal dipolar exchange term. We have analysed the density profiles of the condensate and thermal cloud. In a spherically symmetric trap we can see how the anisotropic dipolar interactions break the spherical symmetry of these density profiles. We show how these results can be interpreted in terms of an effective potential due to direct dipolar interaction term. We calculate the zero-temperature Bogoliubov excitations of the system for a wide range of trap aspect ratios. Due to the limitation on the number of modes we can feasibly include in the calculations, we are limited to very low temperatures. We find that the excitation energies shift very little for these temperatures. The dipolar interactions break the degeneracy between a number of modes.

We then include the thermal dipolar exchange interaction to determine its effect. This term cannot be expressed as an effective potential and it is much more computationally demanding to calculate than the direct dipolar term. We first solve the HFBP equations self-consistently without this term. As long as the effect of the thermal exchange term is small, this will be close to the full solution. We then include the thermal exchange term for a few iterations and find that, in most cases, it is indeed small. This means we can almost reach self-consistency with only a few extra iterations. We measure the importance of the thermal dipolar exchange term by determining the size of its contribution to the chemical potential and we
find that it is about one fifth of the size of the contribution from the direct thermal dipolar term. To examine a situation when the thermal exchange term is relatively large, we look at very small condensate at a temperature where the thermal cloud makes up a significant portion of the system. Here we find that the Bogoliubov excitation energies are shifted up by thermal exchange. In general we find that thermal dipolar exchange has only a small effect on the properties of the condensate. Similar calculations have been performed recently by Ticknor for a quasi-2D dipolar gas [75]. In these calculations he finds that the contribution of thermal dipolar exchange to the chemical potential is about half the size of the direct term. The thermal exchange term therefore appears to be somewhat more important relative to the direct term in two dimensions. He also finds that the total density is strongly affected by thermal dipolar exchange when the temperature is close to the critical temperature. To reach these temperatures in our calculations would require taking into account higher energy thermal atoms with a semiclassical approximation which would require significantly more work.
Appendix A

Derivation of Exchange Term in 2D

The dipolar exchange term with the thermal cloud is given by

$$\Phi_E[x;f(x')] = \int dx' \tilde{n}(x', x)V_{dd}(x' - x)f(x'),$$  \hspace{1cm} (A.1)

where $V_{dd}(x' - x)$ is the dipolar interaction potential. This can be rewritten in the form

$$\Phi_E[x;f(x')] = \frac{1}{(2\pi)^3} \int dk e^{ik \cdot x} V_{dd}(k)f(x,k),$$  \hspace{1cm} (A.2)

where $f(x,k) = \int dx' e^{-ik \cdot x'} \tilde{n}(x', x)f(x')$. While the ground state can be assumed to have no angle-dependent phase, we also want to find solutions of the GPE for larger eigenvalues to use as a basis for solving the BdG equations. Due to the cylindrical symmetry of the problem, these solutions can be assumed to have the form $f(x) = e^{im \phi} f(\rho, z)$. The thermal one body density matrix, $\tilde{n}(x', x)$ also has an angular dependence. It is calculated from the Bogoliubov excitations via equation (4.7),

$$\tilde{n}(x', x) = \sum_{m'} e^{-im'(\rho' - \rho)} \tilde{n}_{m' \rho u}(\rho', \rho, z', z) + e^{im'(\rho' - \rho)} \tilde{n}_{m' \rho u}(\rho', \rho, z', z).$$  \hspace{1cm} (A.3)

We now substitute this into the expression for $f(x, k)$ which gives

$$f(x, k) = \int d\rho' d\phi' dz' \rho' e^{-ik \rho \rho' \cos(\phi' - \phi)} e^{-ikz \phi'} \times \sum_{m'} (e^{-im'(\rho' - \rho)} \tilde{n}_{m' \rho u} + e^{im'(\rho' - \rho)} \tilde{n}_{m' \rho u}) e^{im \phi' f(\rho', z')}.$$  \hspace{1cm} (A.4)
We then change variables to \( \bar{\phi} = \phi' - \phi \), \( k_{\bar{\psi}} = k_{\phi} - \phi \) to give us

\[
f(x, k) = \sum_{m'} \int d\rho' \, dz' \, \rho' e^{-ik_{\bar{\phi}}z'} e^{i\rho \phi}_m f(\rho', z')
\times \left[ \tilde{n}_{m'u} \int d\bar{\phi} \, e^{-ik_{\bar{\phi}}d \bar{\psi} \bar{\phi} - k_{\bar{\psi}} \bar{\phi} e^{-i(m' - m)\bar{\phi}}} + \tilde{n}_{m'v} \int d\bar{\phi} \, e^{-ik_{\bar{\phi}}d \bar{\psi} \bar{\phi} - k_{\bar{\psi}} \bar{\phi} e^{i(m' + m)\bar{\phi}}} \right]. \tag{A.5}
\]

The \( \bar{\phi} \) integrals can be written in terms of Bessel functions so we can write

\[
f(x, k) = 2\pi e^{i\rho} \sum_{m'} e^{-i(m' - m)k_{\bar{\phi}}}\rho \int d\rho' \, dz' \, J_{m' - m}(k_{\rho} \rho') \rho' e^{-ik_{\bar{\phi}}z'} \tilde{n}_{m'u} f(\rho', z')
+ e^{i(m' + m)k_{\bar{\phi}}} \rho \int d\rho' \, dz' \, J_{m' + m}(k_{\rho} \rho') \rho' e^{-ik_{\bar{\phi}}z'} \tilde{n}_{m'v} f(\rho', z'). \tag{A.6}
\]

Using the definition of the Fourier-Hankel transform, (3.53), we write this as

\[
f(x, k) = e^{i\rho} \sum_{m'} e^{-i(m' - m)k_{\bar{\phi}}} \rho \int d\rho' \, dz' \, \tilde{F}\mathcal{H}_{m' - m} \tilde{n}_{m'u} f(\rho', z')
+ e^{i(m' + m)k_{\bar{\phi}}} \rho \int d\rho' \, dz' \, \tilde{F}\mathcal{H}_{m' + m} \tilde{n}_{m'v} f(\rho', z'). \tag{A.7}
\]

Now we can use this \( f(x, k) \) in the expression (A.2) for \( \Phi_E \),

\[
\Phi_E[x; f(x')] = \frac{e^{im\rho}}{(2\pi)^3} \int dk_{\rho} \kappa_{\rho} \int dk_{z} \int dk_{\bar{\phi}} e^{i\rho_{\bar{\phi}} z e^{i\rho_{\bar{\phi}} \cos(k_{\bar{\phi}}) \bar{V}_{dd}(k_{\rho}, k_{z})}
\times \sum_{m'} e^{-i(m' - m)k_{\bar{\phi}}} \rho \int d\rho' \, dz' \, \tilde{F}\mathcal{H}_{m' - m} \tilde{n}_{m'u} f(\rho', z')
+ e^{i(m' + m)k_{\bar{\phi}}} \rho \int d\rho' \, dz' \, \tilde{F}\mathcal{H}_{m' + m} \tilde{n}_{m'v} f(\rho', z'). \tag{A.8}
\]

As before we can write the angular integral in terms of Bessel functions giving us

\[
\Phi_E[x; f(x')] = \frac{e^{im\rho}}{(2\pi)^2} \int dk_{\rho} \kappa_{\rho} \int k_{z} e^{iz} \bar{V}_{dd}(k_{\rho}, k_{z})
\times \sum_{m' = -\infty}^{\infty} \tilde{F}\mathcal{H}_{m' - m} \tilde{n}_{m'u} f(\rho', z') J_{m' - m}(k_{\rho} \rho)
+ \tilde{F}\mathcal{H}_{m' + m} \tilde{n}_{m'v} f(\rho', z') J_{m' + m}(k_{\rho} \rho), \tag{A.9}
\]

which can be written in the form,

\[
\Phi_E[x; f(x')] = \frac{e^{im\rho}}{(2\pi)^2} \int dk_{\rho} \kappa_{\rho} \int k_{z} e^{iz} \bar{V}_{dd}(k_{\rho}, k_{z}) f(\rho, z, k_{\rho}, k_{z}). \tag{A.10}
\]

We can convert the sum over \( m' \) to a sum over only positive \( m' \) in the following
way. The $v$ part of the $m$th contribution to the thermal density matrix is given by

$$ n_{mv}(\rho', \rho, z', z) = v_{jm}(\rho', z') (1 + N_{BE}(E_j)) v^{*}_{jm}(\rho, z). \tag{A.11} $$

Solving the BdG equations for $v_{j,-m}$ is equivalent to using the complex conjugate of the equations so we must have $v_{j,-m} = v_{jm}^*$ and therefore, via (A.11), $n_{m,v}(\rho', \rho, z', z) = n_{m,v}^*(\rho', \rho, z', z)$. We can then combine the positive and negative $m'$ contributions to the sum to give

$$ \tilde{f}(\rho, z, k_{\rho}, k_{z}) = \mathcal{F}_m[H_m^u[(\tilde{n}_{0u} + \tilde{n}_{0v})f(\rho', z')], J_m(k_{\rho}) $$

$$ + \sum_{m'=1}^{\infty} \mathcal{F}_m[H_{m'-m}^u[(\tilde{n}_{m'v}(\rho', \rho, z', z) + \tilde{n}_{m'v}^*(\rho', \rho, z', z)]f(\rho', z')], J_{m'-m}(k_{\rho}) $$

$$ + \mathcal{F}_m[H_{m'+m}^u[(\tilde{n}_{m'u}(\rho', \rho, z', z) + \tilde{n}_{m'u}^*(\rho', \rho, z', z)]f(\rho', z')], J_{m'+m}(k_{\rho})]. \tag{A.12} $$
Bibliography


