The Hartree-Fock-Bogoliubov Theory
of
Bose-Einstein Condensates

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Abstract

In this thesis we develop an orthogonalised Hartree-Fock-Bogoliubov (HFB) formalism that has a zero-energy excitation (in contrast with standard HFB). We demonstrate that this formalism satisfies the number and linear/angular momentum conservation laws (as does standard HFB). This formalism is applied to vortices in 2D Bose-Einstein condensates (BECs) in axially-symmetric harmonic traps, where we initially find solutions for on-axis vortices, determining the energy spectrum and hence the lowest core localised state (LCLS) energy. In the $T = 0$ case we identify this with the anomalous mode which gives a zero excitation energy in the frame rotating at this frequency. For this reason the anomalous mode frequency was identified in the earlier literature with the precessional frequency for an off-axis vortex. However the LCLS energy is positive in the finite temperature case. Hence, associating this LCLS energy with the precessional frequency leads to the erroneous conclusion that the vortex precesses in the opposite direction to the $T = 0$ case, which is clearly physically unreasonable. In order to address this problem, we derive an equation for the prediction of vortex precessional frequencies from the continuity equation, and use this equation solved self-consistently with the orthogonal HFB equations in the frame rotating at this predicted frequency to create off-axis vortices at pre-specified positions. Hence we are able to predict the precessional frequencies and show that these are consistent with the $T = 0$ case, and are entirely unrelated to the LCLS energy. We also consider a two-state model and demonstrate that this model is insufficient for the description of single off-axis precessing vortices. We formulate a generalised multi-state model, using the normalisation conditions for the model to derive an equation predicting the precessional frequency of the vortex, and demonstrate equivalence with the continuity equation prediction. We use the time-dependent HFB equations to simulate creation of vortices by stirring the BEC by means of a Gaussian optical potential, finding very good agreement of the measured precessional frequencies of the vortices in stirred BECs with the predicted values. We find the existence of a critical stirring frequency for the creation of vortices in regions of appreciable superfluid density, in qualitative agreement with experiment. We then investigate the consequences of breaking rotational symmetry and find that breaking the axial symmetry of the harmonic trapping potential leads to loss of angular momentum, and hence to the decay of vortices. Finally we develop a finite temperature treatment of the Bose-Hubbard model based upon the Hartree-Fock-Bogoliubov formalism in the Popov approximation to study the effect of temperature upon the superfluid phase of ultracold, weakly interacting bosons in a one-dimensional optical lattice.
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Glossary

BEC  Bose-Einstein condensate
GPE  Gross-Pitaevskii Equation
HFB  Hartree-Fock-Bogoliubov
GGPE  Generalised Gross-Pitaevskii Equation
BdGE  Bogoliubov deGennes Equations
$U(\mathbf{r} - \mathbf{r}')$  2-body bare interaction potential
$g\delta(\mathbf{r} - \mathbf{r}')$  Contact potential approximation
$g \equiv 4\pi\hbar^2a_s/m$  Interaction strength associated with contact potential approximation
$\hat{\psi}(\mathbf{r},t)$  Bose field operator
$V_T(\mathbf{r})$  Trapping potential
$\hat{h}(\mathbf{r})$  Single-particle Hamiltonian
$\hat{h}_\Omega(\mathbf{r})$  Single-particle Hamiltonian in frame rotating with angular frequency $\Omega$
$\hat{b}_k, \hat{b}_k^\dagger$  Creation and annihilation operators for a particle in state $k$
$\hat{H}(t)$  Bose Hamiltonian
$\mu$  Chemical potential of Bose-Einstein condensate
$\hat{H}^{(GC)}(t)$  Grand-Canonical Bose Hamiltonian
$\Phi(\mathbf{r},t)$  Condensate wave function
$\hat{\eta}(\mathbf{r},t)$  Fluctuation operator in Bogoliubov decomposition
$\hat{H}_{\text{HFB}}(t)$  HFB approximation to the Grand-Canonical Hamiltonian $\hat{H}^{(GC)}(t)$
$\tilde{n}(\mathbf{r},t)$  Thermal density $\tilde{n}(\mathbf{r},t) \equiv \langle \hat{\eta}^\dagger(\mathbf{r},t)\hat{\eta}(\mathbf{r},t) \rangle$
$\tilde{m}(\mathbf{r},t)$  Anomalous density $\tilde{m}(\mathbf{r},t) \equiv \langle \hat{\eta}(\mathbf{r},t)\hat{\eta}(\mathbf{r},t) \rangle$
$N_{\text{BE}}(\epsilon_q)$  Bose-Einstein distribution for excitation energy $\epsilon_q$
$N$  Total number of atoms in BEC
$N_c$  Total number of condensate atoms in BEC
$\tilde{N}$  Total number of non-condensate atoms in BEC
$F_c$  Condensate fraction, $F_c \equiv N_c/N$
$\tilde{F}$  Non-condensate fraction, $\tilde{F} \equiv \tilde{N}/N$
Temperature of BEC

Condensate to normal gas transition temperature

Creation and annihilation operators for \( q^{th} \) quasi-particle energy mode

Amplitudes associated with \( q^{th} \) quasi-particle energy mode

On-diagonal operator in BdGEs in Bogoliubov approximation

Off-diagonal operator in BdGEs in Bogoliubov approximation

On-diagonal operator in BdGEs for standard HFB formalism

Off-diagonal operator in BdGEs for standard HFB formalism

Condensate effective interaction for G1 and G2 gapless approximations

Non-condensate effective interaction for G1 and G2 gapless approximations

On-diagonal operator in BdGEs for gapless HFB approximation

Off-diagonal operator in BdGEs for gapless HFB approximation

On-diagonal operator in BdGEs for Popov approximation

Off-diagonal operator in BdGEs for Popov approximation

Projection operator in orthogonal GGPE that maintains linear and angular momentum conservation

Projection operator in orthogonal BdGEs that maintains orthogonality of condensate and non-condensate

On-diagonal operator in BdGEs for orthogonal HFB formalism

Off-diagonal operator in BdGEs for orthogonal HFB formalism

Normal correlation density \( \tilde{n}(r, r', t) \)

Anomalous correlation density \( \tilde{m}(r, r', t) \)

On-diagonal operator in BdGEs for orthogonal HFB formalism with quasi-particle energy shift \( \Delta \epsilon \)

On-diagonal operator in BdGEs for perturbed orthogonal HFB formalism for quasi-particle energy \( \epsilon_q \)

Off-diagonal operator in BdGEs for perturbed orthogonal HFB formalism for quasi-particle energy \( \epsilon_q \)

\( n^{th} \) eigenvalue of GGPE

\( n^{th} \) eigenstate of GGPE

Single-particle eigenvalue (corresponding to single-particle Hamiltonian \( \hat{h}(r) \)) of mode \( k \)

Single-particle eigenvalue (corresponding to single-particle Hamiltonian \( \hat{h}_{\Omega}(r) \)) of mode \( k \)

Single-particle eigenstate (corresponding to single-particle Hamiltonian \( \hat{h}(r) \)) of mode \( k \)
Radial and axial trapping frequencies in axially symmetric harmonic trap

Aspect ratio \( \lambda \equiv \omega_z / \omega_r \) in axially symmetric harmonic trap

Length scale \( r_0 = \sqrt{\hbar / m \omega_r} \) in axially symmetric harmonic trap

Time scale \( t_0 = 2 / \omega_r \) in axially symmetric harmonic trap

Energy scale \( t_0 = 2 / \omega_r \) in axially symmetric harmonic trap

Interaction strength in 3D harmonically confined BEC system in dimensionless units of \( r_0, t_0, \) and \( E_0 \) as defined,

\[
C_{3D} = 8 \pi (a_s / r_0) N
\]

Interaction strength for quasi-2D BEC system in harmonic trap with tight axial confinement in dimensionless units of \( r_0, t_0, \) and \( E_0 \) as defined,

\[
C_{2D} = 8 \pi \left( \frac{\lambda}{2 \pi} \right)^{1/2} (a_s / r_0) N
\]

Condensate to normal gas transition temperature for ideal 2D gas

Interaction strength in tightly axially confined harmonically confined axially symmetric BEC system where the angular coordinate \( \theta \) has been integrated out, so the system is effectively 1D in the radial coordinate \( r \),

\[
C_{2D}^R = 4 \left( \frac{\lambda}{2 \pi} \right)^{1/2} (a_s / r_0) N
\]

Laguerre basis functions defined for \( (l, n) \in S \) where

\[
S \equiv \{ l, n \mid n = 0, \ldots, l = 0, \pm 1, \ldots \}
\]

Set of all possible quantum numbers for modified Laguerre basis functions for a single off-axis vortex defined by

\[
S^{(1)} \equiv \{ l, n \mid (l, n) \in S - \{(1,0)\} \}
\]

Set of all possible quantum numbers for modified Laguerre basis functions for \( N_v \) off-axis vortices defined by

\[
S^{(N_v)} \equiv \{ l, n \mid (l, n) \in S - \{(1,0), \ldots, (N_v,0)\} \}
\]

Modified Laguerre basis functions specifying the position of a single off-axis vortex

Modified Laguerre basis functions specifying the position of \( N_v \) off-axis vortices

Out-coupling potential

Second-order coherence function
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Chapter 1

Introduction

1.1 Overview of Bose-Einstein Condensates

Microscopic particles in nature are of two types - those having an integral spin, called Bosons, and those having half-integral spin, fermions. The consequences of this are profound in systems consisting of many such particles. The laws of quantum mechanics imply that the overall wave-function of a system of identical particles be symmetric in the case of Bosons or anti-symmetric in the case of fermions. Familiar sub-atomic particles such as protons, neutrons, and electrons are all fermions and obey the Pauli exclusion principle, which precludes any two fermions occupying identical quantum states. This is responsible for the chemistry of atoms as reflected in the familiar periodic table of the elements. Without the Pauli exclusion principle, such chemical properties would not exist, and hence life as we know it would not be possible. Another important consequence lies in the existence of a surface in momentum space known as the Fermi surface due to the systematic filling of energy levels, two per energy level, one for spin up and one for spin down, found in crystalline structures. The magnitude of the Fermi energy relative to the energy bands of the structure determines whether a material is an insulator, a semi-conductor or a conductor.

Bosons on the other hand do not obey the Pauli exclusion principle, and at sufficiently low temperatures, it becomes over-whelmingly favourable for a very large number of atoms to occupy the ground state. Such a phenomenon occurs when dilute Bose gases (i.e. gases of atoms/molecules composed of an even number of sub-atomic particles) are cooled below the transition temperature, and is known as Bose-Einstein condensation, in honour of the Indian physicist Bose who first derived the theory of the quantum statistics of integral
spin particles, and to Einstein who was instrumental in getting this work published, and who first predicted the phenomenon of Bose-Einstein condensation in 1924. Associated closely with Bose-Einstein condensation is the notion of superfluidity. Superfluidity was first observed in liquid helium where rotational motion persists without dissipation, and is accompanied by multitudes of quantised vortices with minute cores owing to the strong interactions in liquid helium. Superconductivity, the unimpeded flow of current in a superconducting material, observed in certain materials at temperatures below the transition point, is closely related to superfluidity, and was first observed by Kamerlingh Onnes in 1911, even earlier than superfluidity in liquid helium.

Due to the extremely low transition temperatures associated with Bose-Einstein condensation, the first dilute, weakly interacting Bose-Einstein condensate (BEC) was produced only years later in 1995 by Anderson et. al. [1]. The advent of the creation of BECs produced much excitement for several reasons.

Firstly, the macroscopic occupation of a single quantum state allows us to investigate quantum phenomena on a macroscopic level. At such low temperatures, the de Broglie wavelength is comparable with the size of the BEC, hence all atoms in the BEC are coherent and therefore exhibit wave-like features. For example, two interacting BECs produce an interference pattern analogous to two interfering laser beams. As a consequence of the coherence of the atoms, the hydrodynamics of a BEC fluid differs from that of a conventional fluid in that vortex production is only possible if accompanied by a discontinuity in the phase in multiples of \(2\pi\), and hence the circulation of a BEC fluid is quantised in multiples of \(2\pi\). This necessitates a vanishing density at some point in the core of the vortex. A vortex in a BEC is in some way analogous to the quantised flux lines associated with superconductors, and is therefore of considerable theoretical interest.

Secondly, since the interactions in BEC systems are weak in view of the diluteness of the gases, BECs allow us to model other systems in Physics, such as crystal lattices, which, due to strong interactions and the presence of impurities and dislocations, are extremely messy and very difficult to model. Using counter-propagating detuned laser beams, one is able to create periodic potentials, and to load BECs into the potential wells associated with these periodic potentials. In this way one is able to model a crystalline lattice. By varying the depth of the potential wells, one can alter the tunnelling potential between adjacent lattice sites. In the limit of low tunnelling potential, one can create a superfluid within the optical lattice below a transition temperature \(T_c\). At the other extreme, one can make the tunnelling potential sufficiently high that, for all intents and purposes, the optical
lattice behaves as an insulator. This is known as the Mott insulator regime. One can also introduce optical speckle or a laser potential of incommensurate frequency with the lasers producing the optical lattice, thus modelling random potentials representing impurities. In this way, one is able to observe Anderson localisation in optical lattices. Optical speckle can also be introduced into a BEC confined by a single harmonic potential, and Anderson localisation effects observed provided the optical speckle is of suitably small dimensions.

1.2 This work

In this thesis we shall be concerned with the study of vortices in quasi-2D BECs and with superfluidity and the BEC transition temperature in 1D optical lattices. A BEC is essentially an ensemble of identical particles which are predominantly all in the same (ground) state. At zero temperature for a 3D Bose gas, one may, for all intents and purposes, assume that all the particles are in the ground state, and hence the system may be treated using a single particle wave equation with two-body interactions, namely the non-linear Schrödinger equation, otherwise known as the Gross-Pitaevskii equation. At finite temperature, and in lower-dimensional systems, the situation is somewhat more complicated. Solving the many-body Schrödinger equation is essentially an intractable problem, except for very small systems, since the many-body wave-function is composed of every possible symmetric permutation of the products of the single-particle wave-functions in the case of Bosons, and of anti-symmetric permutations in the case of Fermions. For the systems considered here, this is completely impractical, and so another approach to the problem must be found. One possible approach consists of representing the problem in terms of creation and annihilation operators for the kets of every possible occupation number of every possible state. These kets span a space known as Fock space, which is an infinite-dimensioned vector space. The problem is still intractable, however, and approximations need to be made in order to solve this problem. The approach used here, known as the Hartree-Fock-Bogoliubov formalism, makes the assumption that most of the atoms are in the same (ground) state and that these atoms may be represented classically in the form of a complex-valued wave-function (the condensate wave-function), and treats the remainder as excitations of the ground state by means of a fluctuation operator. The assumption is then made that these excited atoms (non-condensate) may be represented as collective excitations in the form of non-interacting quasi-particles. To do this, one assumes that such a quasi-particle basis exists, and makes a canonical transformation, known as the Bogoliubov transformation. The condensate wave-function then obeys a wave equation
similar to the Gross-Pitaevskii equation, but with the effects of the non-condensate now included. The transformation amplitudes for the quasi-particle creation and annihilation operators satisfy the Bogoliubov-de Gennes equations. These equations are collectively known as the Hartree-Fock-Bogoliubov equations.

The problem with this approach is that in assuming the presence of a condensate, the $U^{(1)}$ symmetry is broken. This implies by the Hugenholtz-Pines theorem, that there must exist a zero-energy quasi-particle. This is known as the Goldstone mode, and implies that the energy spectrum must be gapless. Unfortunately in the above decomposition of the Bose field into a classical field, and a fluctuation operator which itself is represented in terms of a non-interacting quasi-particle basis, and in taking quantum expectation values (the mean-field approximation), the condensate and non-condensate are treated inconsistently, resulting in a non-zero lowest energy excitation, and hence a gap in the excitation energy spectrum. Since there is no zero-energy excitation, this implies there is no Goldstone mode, and therefore the Hugenholtz-Pines theorem is violated. However, since this theory is also a variational theory, and hence a conserving theory, all the physical conservation laws, for example number, both linear and angular, and energy conservation, are satisfied. The energy gap problem may be corrected in one of several ways by making a further approximation. In the so-called Popov approximation, the anomalous density is ignored. This is justified along the lines that two-body collisions are double-counted when one takes into account the 2-body T-matrix. The result of this approximation is that the energy spectrum is now gapless, however the number, both angular and linear momentum, and energy conservation laws are violated in the time-dependent case, and therefore this is an unsuitable formalism for the time-dependent simulations performed here. It is also unsuitable in the prediction of precessional frequencies of BEC systems with one or more off-axis vortices, since the continuity equation is invalid in view of number conservation violation. The so-called G1 and G2 gapless approximations (see later) replace the bare interactions with the many-body T-matrix in the low momentum limit, and this also remedies the problem with the energy gap, but still violates the number, both angular and linear momentum, and energy conservation laws. Therefore none of these theories are suitable for the work to be undertaken in this thesis.

Here we develop and use an orthogonalised HFB formalism which, whilst it does not correct the excitation spectrum, nevertheless allows for a zero-energy excitation. We also develop perturbation theory by which the excitation spectrum may be corrected, thus we obtain a gapless theory, which is also conserving (i.e., obeys the number, both the angular and linear momentum, and energy conservation laws). This has not been used in the results
presented here, since it was not available at the time, but some calculations done here reveal that these perturbative corrections do not significantly affect the results of this thesis.

When one solves the GPE for an on-axis vortex, one finds that the Bogoliubov spectrum has a lowest-lying energy that is negative, the so-called anomalous mode. The lowest-lying energy is zero in the frame rotating at this frequency, leading one to conclude that this is the precessional frequency of the vortex.

Solving the HFB equations for an off-axis vortex at finite temperature in the Popov approximation (or in the case of the G1 or G2 approximations) in a regime having sufficiently strong interactions in the finite-temperature case, however, yields a (small) positive lowest lying energy mode, the so-called lowest core localised state (LCLS), and this can be generalised to a lower bound for the LCLS energy for an off-axis vortex. It was argued that, in both cases, the thermal cloud acts as an effective potential, thereby stabilising the vortex, but this fails to take into account the dynamics of the thermal cloud itself. The association of this energy with the precessional frequency [2, 3] leads to the conclusion that the vortex precesses in the direction opposite to the condensate flow around the core. This is inconsistent with experiment, and also seems intuitively unreasonable, since zero-temperature predictions would suggest otherwise, and one might reasonably expect continuous variation with temperature. Later finite-temperature calculations for off-axis calculations for off-axis vortices [4] do, however, conclude that no correlation exists between the precessional frequency and the anomalous mode.

In this thesis we demonstrate that there is no correlation between the LCLS energy and the precessional frequency. To simplify the calculation, we consider a quasi-two-dimensional BEC trapped by means of an axially-symmetric harmonic potential, where the axial confinement is sufficiently strong such that all the excited axial states can be neglected, but not strong enough to affect the scattering, which is still effectively 3D. This effectively reduces the problem to a 2D problem. We note that the solutions to the HFB equations for an off-axis vortex are stationary in the frame rotating about the axis of symmetry of the harmonic trapping potential at the precessional frequency of the vortex. This precessional frequency is predicted making novel use of the continuity equation for the condensate density. The HFB equations are then solved self-consistently in the rotating frame with this equation for the vortex precessional, and the position of the vortex is incorporated to the basis representation for the condensate wave-function. Thus off-axis vortices can be created at any position, provided the vortex position does not lie on any of the roots of the basis functions. We thus establish that the precessional frequencies of the vortex
at various positions and at various temperatures are uncorrelated with the corresponding LCLS energies. We obtain results for on-axis vortices by extrapolation of the data, and verify this by on-axis calculations solved in the frames rotating at the corresponding extrapolated precessional frequencies, obtaining the same LCLS energies as the extrapolated LCLS energies, and likewise conclude that no correlation exists between the extrapolated rotational frequencies and the LCLS energies for the on-axis case.

We extend this to multiple vortex arrays. Thus we are able to predict the precessional frequencies of vortices, not only for single off-axis vortices, but also for vortex arrays consisting of two vortices, and of triangular (three vortices) and hexagonal (seven vortices) vortex arrays for varying off-axis distances or lattice parameters at various temperatures up to \( \sim \frac{T_c}{2} \) where \( T_c \) is the transition temperature of the BEC. We test these predictions in time-dependent simulations, including simulations of stirred condensates. We also note in these simulations that the conservation laws are satisfied, as one would expect, since HFB is a variational, and hence a conserving theory. We shall therefore be concerned with an orthogonalised HFB theory, and will demonstrate that this is also a conserving theory.

In chapter 2 we review the theoretical background for such a treatment, and commence with the equivalence between the first and second quantised representations of the quantum many-body problem. We then investigate various approaches in solving the many-body problem in the second quantised form, focussing mainly on number-conserving and symmetry-breaking mean-field theories. Since coherent states do not have well-defined number eigenstates, symmetry-breaking mean-field formalisms violate number conservation, but introducing a chemical potential as a Lagrange multiplier, and working in the Grand-Canonical Ensemble ensures that particle number is conserved. In the symmetry-breaking approach we split the Bose field operator into a c-field part representing the condensate, and a fluctuation operator part. To lowest order we neglect the thermal part and obtain the Gross-Pitaevskii Equation (GPE) [5–9] which is a \( T = 0 \) theory. If we excite the condensate and retain perturbation terms to lowest order, we can calculate the collective excitations of the condensate (linear response theory), and these equations correspond to the Bogoliubov-de Gennes equations (BdGEs) in the Bogoliubov approximation. In deriving the BdGEs we transform the thermal part (the fluctuation operator) into a basis of non-interacting quasi-particles representing the elementary excitations, and this is justified with its correspondence at \( T = 0 \) (Bogoliubov approximation) to the linear response theory [6–10]. At finite temperature we obtain the Hartree-Fock-Bogoliubov (HFB) equations [11] which suffer from various theoretical problems, not least of which is the unphysical gap in the quasi-particle spectrum, and hence the violation of the Hugenholtz-Pines theo-
rem. To get around this problem, we can make various approximations to obtain gapless theories which rectify this situation, but unfortunately these lead to violation of important conservation laws. The theories discussed here, may be divided into two categories:

1. Symmetry-breaking Mean-Field Theories, and
2. Number-conserving Theories.

**Symmetry-breaking Mean-Field Theories** The symmetry-breaking mean-field theories discussed here are:

1. The Gross-Pitaevskii Equation (GPE) [5–9] where the Bose field operator is regarded as a mean-field, and replaced by a c-number. This represents the Hamiltonian to zeroth order, and yields the GPE. The excitations can be found using linear response theory [6–10] yielding the Bogoliubov-de Gennes Equations (BdGEs) in the Bogoliubov approximation,

2. The Hartree-Fock-Bogoliubov (HFB) Formalism [11] where the Bose field operator is separated into a condensate and a thermal fluctuation operator which is decomposed into a basis of non-interacting quasi-particles using a Bogoliubov transformation. The condensate part is considered to be a mean field, and is represented by a c-field. Thus the $U(1)$ symmetry of the Hamiltonian is broken, leading to violation of particle conservation. However, this problem may be overcome by considering the Grand-Canonical Hamiltonian, where the chemical potential $\mu$ is introduced as a Lagrange multiplier, thereby ensuring particle conservation. This leads to the HFB equations consisting of a generalised Gross-Pitaevskii equation (GGPE) for the condensate, and a set of BdGEs for the quasi-particle amplitudes. The HFB formalism is a conserving theory, i.e. the conservation laws are satisfied, but the symmetry-breaking has various problems, one of which is an unphysical gap in the quasi-particle energy spectrum, violating the Hugenholtz-Pines theorem [11], and the Grand-Canonical catastrophe [12, 13]. In view of the approximations concerning the mean-field, HFB theory is valid for low temperatures, typically for $T \lesssim T_c/2$, where $T_c$ is the transition temperature.

3. The Popov Approximation to HFB\(^1\) [11] addresses the energy gap problem by ignoring the anomalous density, arguing that two-body correlations are represented by

\(^1\)An objection to this terminology has been raised by Yukalov [14].
the anomalous density \( \tilde{m} \), and therefore the s-wave scattering length \( a_s \) is already measured in the presence of two-body collisions (correlations) [15–17]. In order to understand this we note that the contact potential approximation \( U(r - r') = g\delta(r - r') \) used here\(^2\), where \( g \) is the interaction strength given by \( g = 4\pi\hbar^2 a_s/m \), represents an approximation to the 2-body T-matrix, and not to the full 2-body bare interaction potential \( U(r - r') \). Using this approximation, one achieves a gapless quasi-particle energy spectrum. However, as we shall see in chapter 4, the number and linear/angular momentum conservation laws are violated.

4. The G1 and G2 Gapless Theories [15–17, 19, 21] allows one to proceed beyond the two-body T-matrix. This can be achieved by replacing the contact potential approximation to the two-body T-matrix in the GPE and in the BdGEs in the Bogoliubov approximation by the expression \( g \left( 1 + \frac{\tilde{m}(r)}{\Phi(\mathbf{r}, t)} \right) \), where \( \tilde{m} \) is the anomalous density defined in chapter 2, equation (2.60) and \( \Phi \) the condensate wave-function (see section 2.6.1). Thus we introduce the anomalous density \( \tilde{m} \) into the formalism. As in the case of the Popov approximation, one achieves a gapless quasi-particle energy spectrum. However the number and linear/angular momentum conservation laws are again violated. This is discussed in more detail in chapter 4.

**Number-conserving Theories** The number-conserving mean-field theories discussed here are:

1. The formalism proposed by C. W. Gardiner [22], which is a \( T = 0 \) theory, and essentially yields the GPE, where the excitations for quasi-particle modes may be

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\(^2\)For dilute gases at very low temperature, it is customary to assume that collisions between two atoms are perfectly elastic local collisions, and hence can be treated in the same way as two colliding billiard balls, and hence that the approximation \( U(r - r') = g\delta(r - r') \) for the full 2-body inter-atomic potential can be applied. Since the gas is dilute and at very low temperature, only the asymptotic scattering states are important, thus the only effect of atomic interactions in these states is a change of phase in the wave-function. This phase change can be well approximated by a pseudopotential of the form [18] \( V_{\text{pseudo}}(r) = g\delta(r)\frac{\partial}{\partial r} r \rightarrow g\delta(r) \). However this approximation is only valid for low momenta, and inclusion of high momenta states leads to ultra-violet divergence due to the use of a constant interaction strength with an unrestricted summation over momenta. This also leads, in effect, to double counting. This problem can be overcome by a suitable re-normalisation, which is tantamount to upgrading the exact interatomic potential to an effective interaction given by the T-matrix. The contact approximation can then be seen as an s-wave approximation to the 2-body T-matrix, and not the full 2-body inter-atomic potential - see also discussion in [5].
determined using the BdGEs in the Bogoliubov approximation in its number con-
serving generalisation,

2. The formalism proposed by S. A. Morgan [23,24], which is a finite temperature theory
using first order perturbation theory to take into account the quadratic terms in the
thermal fluctuation operator, and second-order perturbation to determine the energy
shifts due to the higher order terms. This yields a set of equations consisting of the
GGPE (as in HFB theory), and a modified set of BdGEs where the Hamiltonian is no
longer diagonalisable in terms of the quasi-particle energies (as is the case in HFB),
but where there is dependency on the excitation energy in the BdGEs for each of the
quasi-particle modes,

3. The formalism proposed by Y. Castin and R. Dum [25] where a number-conserving
approach (together with an appropriate form for the fluctuation operator) is used
to obtain a systematic expansion of the Hamiltonian. The dynamical equations are
then derived for the condensate and the quasi-particle amplitudes to various orders.
To first order, the GPE is recovered, with the quasi-particle amplitudes described by
the BdGEs in the Bogoliubov approximation. Subsequent orders yield higher order
corrections to these equations. This formalism is discussed in more detail in chapter
2,

4. The formalism proposed by S. A. Gardiner et. al. [26] where a number-conserving
approach is used along similar lines to Y. Castin and R. Dum [25], but where they
choose a slightly different fluctuation operator, again obtaining a systematic expa-
sion of the Hamiltonian. The dynamical equations are then derived for the condensate
and the quasi-particle amplitudes to various orders yielding a generalised form for
the GPE, and a set of modified BdGEs. This formalism is discussed in more detail
in chapter 2, where some of the problems with this formalism are examined.

Other problems associated with the HFB formalism are the fact that the condensate and
non-condensate quasi-particle amplitude wave-functions are not orthogonal, and the so-
called Grand-Canonical catastrophe. These issues are discussed in chapter 2, and later in
chapter 4. We also consider briefly in chapter 2, two other approaches, namely, the pro-
jected Gross-Pitaevskii (PGPE) [27,28] and the truncated Wigner [27,29–32] approaches.

In the classical field approach [27,28] we look to describe the modes within a BEC by
means of classical fields. The assumption is that all such modes are highly occupied, an
assumption that is only likely to be valid provided the temperatures are not too low. Such
methods are very useful in describing quasi-condensates (where the mean-field methods are not generally applicable), and in other areas where the mean-field theories break down. There are many approaches possible, one of which is the approach due to Davis, Morgan and Burnett [28] wherein the non-linear term $|\phi|^2 \phi$ in the GPE is replaced by $\hat{P} \{ |\phi|^2 \phi \}$, where $\hat{P}$ is a projection operator that projects the non-linear term into the set of basis states below an energy cut-off point, i.e. into the so-called condensate band. This approach leads to one of several variants of the PGPE.

In the truncated Wigner approach [27, 29–32] we expand the Hamiltonian in a restricted basis set. Using the multi-mode Wigner function, we can establish for the von Neumann equation a set of correspondences between the creation and annihilation operators and derivatives of the Wigner function. This yields a third order differential equation. By retaining only first-order derivatives (we discard all terms involving third order derivatives), one is able to establish a correspondence between the Fokker-Planck equation governing the evolution of this multi-mode distribution and a stochastic differential equation which describes Gaussian random fluctuations around the drift evolution. This eventually yields an equation that is similar to the PGPE, however the PGPE formalism is applicable to scenarios of high temperatures $\sim 3T_c/4 \rightarrow T_c$, whereas the truncated Wigner approach is essentially a $T = 0$ theory in view of the truncation of the von Neumann equation. These formalisms will be discussed again briefly in chapter 2.

In chapter 3 we present a brief survey on vortices in BECs. Topological defects occur as a result of phase-discontinuities in the BEC, examples of which are vortices, which have a phase circulation about the point of zero density with a corresponding phase discontinuity of a multiple of $2\pi$ - usually $2\pi$ because multiply-charged vortices are very unstable and soon break up into singly charged vortices. Vortices may be produced in BECs in several different ways, some of which are:

1. Phase-imprinting wherein a phase is imprinted on the BEC by means of a polarised laser beam,

2. By cooling a rotating thermal cloud which forms a BEC with vortices when cooled,

3. By simply stirring a condensate by means of a dipole optical potential.

In Chapter 4 we develop further the theory for the HFB formalism and introduce an orthogonal HFB formalism which allows for a zero energy excitation, in contrast to the
standard HFB formalism. However, the existence of a zero energy eigenvalue does not imply that the Hugenholtz-Pines theorem [11] is satisfied, or indeed that this corresponds to the Goldstone mode, nor is the remainder of the energy spectrum “corrected”, and is quite similar to the standard HFB spectrum in spite of the existence of a zero energy eigenvalue. We demonstrate this in section 4.3.1 where we show the existence of a null subspace of zero-energy eigenvalue modes for the orthogonal BdGEs spanned by the mode \((\phi, -\phi^*)\), where \(\phi = \Phi/\sqrt{N_c}\), with \(\Phi\) the condensate wave-function, and \(N_c\) the number of condensate atoms, (i.e. \(\phi\) is normalised to unity). We show in sections 4.3.3-4.3.5 that the physical conservation laws of particle, energy and angular momentum conservation are still satisfied, and present in section 4.3.8 perturbation calculations by which the quasi-particle spectrum might be corrected, thus yielding a gapless theory in which all important conservation laws are satisfied. In section 4.3.6 we derive an equation predicting the precessional frequencies of off-axis vortices (including vortex arrays, provided the vortices are not too close), using the continuity equation for the condensate density, which is then solved self-consistently with the time-independent orthogonal HFB equations in the frame rotating at the vortex precessional frequency.

In chapter 5 on numerical methods, we explore methods by which the time-independent and time-dependent calculations may be performed, including the calculation of the precessional frequencies of vortices.

In chapter 6 we simulate the evaporative cooling of 2D BECs in axially-symmetric harmonic traps using time-dependent HFB theory, and use time-independent HFB theory to estimate the effective temperature at various times during the evaporative cooling process. We find that the system equilibrates to a reasonable approximation provided the cooling process is not too rapid. We find, however, no evidence of condensate growth, although cooling of the condensate is achieved. This is due to the fact that significant damping processes (probably the Landau and Beliaev processes) are not accounted for in HFB due to the application of Wick’s theorem for ensemble averages. In HFB the fluctuation operator is expanded in terms of a non-interacting quasi-particle basis (see next chapter). Since the ensemble average of odd powers of the quasi-particle creation and annihilation operators is zero, the terms involving the Beliaev and Landau processes are zero in the HFB mean-field approximation.

In chapter 7 we investigate vortices in 2D BECs in axially-symmetric harmonic traps using orthogonal HFB theory developed in chapter 4. In section 7.2 we find solutions for on-axis vortices, determining the energy spectrum and hence the lowest excitation energy, referred
Chapter 1. Introduction

to in the literature as the lowest common localised state (LCLS) energy [2,3]. In the $T = 0$ case we identify this with the anomalous mode which, when we transform to the frame rotating at the frequency corresponding to this energy, gives a zero excitation energy. For this reason the anomalous mode frequency was identified in the earlier literature with the precessional frequency for an off-axis vortex [36–41]. This led to the misconception that the LCLS energy in the finite temperature case corresponded to the precessional frequency for an off-axis vortex, and hence to the erroneous conclusion that the vortex precessed in the opposite direction to the $T = 0$ case [2,3]. We show in section 7.4 that the precessional frequency for an off-axis vortex (or for several off-axis vortices) may be predicted using the continuity equation for the condensate density, and solved self-consistently with the Hartree-Fock-Bogoliubov (HFB) equations. We show that these predicted precessional frequencies are consistent with the $T = 0$ case, and are entirely uncorrelated with the LCLS energy. In section 7.3.1 we create an off-axis vortex using the two-state model, and we see that this model is only valid for extremely weak interactions, and breaks down rapidly as we increase the interactions, becoming meaningless at the interaction strengths considered here (which are only moderate). In sections 7.3.2 and 7.3.3 we generalise the two-state model to a generalised multi-state model and use the normalisation conditions for the model to derive an equation predicting the precessional frequency of the vortex. We don’t solve these equations self-consistently, but show in section 7.4.4 the equivalence of the multi-state model with the method described in section 7.4.1 where we specify the position of the vortex using modified basis functions\(^3\) for the condensate wave-function and solve the HFB equations self-consistently in the frame rotating at the precessional frequency predicted by the continuity equation for the condensate density. We find numerically (see figure 7.13) that there is excellent agreement between the two predictions provided the mode cut-off is sufficient. In section 7.4.3 we also calculate the precessional frequencies for two vortices, and triangular and hexagonal vortex arrays, and the precessional frequencies are compared in figure 7.12.

In section 7.5.2 we use the time-dependent HFB equations to create vortices by stirring the BEC by means of a Gaussian optical potential, and in section 7.5.3 to examine the conservation of angular momentum and how breaking the axial symmetry of the harmonic trapping potential leads to loss of angular momentum, and hence to the decay of vortices. We find very good agreement of the measured precessional frequencies of the vortices

\(^3\)The modified basis functions are defined in terms of the single-particle basis functions and depend on the vortex position. This can be extended by an iterative process to any number of vortices, and makes it easy to place the vortices in any position provided this does not fall on any root of the single-particle basis functions.
in stirred BECs with the predicted values in section 7.4.3. In section 7.5.2 we find the existence of a critical stirring frequency (corresponding to a velocity of the stirring potential through the fluid of just slightly in excess of the Landau critical velocity), below which no vortices are created in regions of appreciable superfluid density (i.e. within the Thomas-Fermi radius). This is in qualitative agreement with work done by Dalibard et. al. [42].

Noether’s theorem states that in a conservative system, a differentiable symmetry of the Lagrangian has a conserved quantity associated with the system. In the case of an axially symmetric trapping potential, therefore, we would expect the axial component (i.e. the z-component) of the angular momentum to be conserved. This is indeed found to be the case, and in section 7.5.3 we investigate the consequences of breaking this symmetry. We predict that angular momentum should be lost, and hence the vortex/vortices in a rotating condensate should decay. Simulations in section 7.5.3 reveal that this is indeed the case, and we observe the decay of vortices in BECs in two cases, namely for a BEC containing a single precessing off-axis vortex, and for a BEC containing a precessing triangular vortex lattice.

In chapter 8 we apply finite temperature mean-field theory of BECs in 1D optical lattices using the Bose-Hubbard model in the Popov approximation. We calculate the superfluidity of the BEC in a 1D optical lattice in two situations:

1. No trapping potential (periodic boundary conditions),
2. In the presence of an underlying harmonic trapping potential.

In both cases we extrapolate the superfluidity calculations as a function of temperature to estimate a superfluid-normal fluid transition temperature.

1.3 Peer-reviewed Publications

Some of the work presented in this thesis has been published in peer-reviewed journals.

- The work on the Finite Temperature Theory of Ultra-cold Atoms in a One-dimensional Optical Lattice covered in chapter 8 appears in Physical Review A [43] where the transition from the superfluid phase to the normal fluid phase is investigated, both for the untrapped case, and the harmonically trapped case.
• The work on the Precession of Vortices in dilute Bose-Einstein Condensates at finite Temperature (see chapter 7) may be found in Physical Review A [44] and includes predictions for the precessional frequencies of single off-axis vortices in BECs. This work also touches briefly on calculations for a triangular vortex array.

• A paper consisting of the development of the theory for the orthogonal HFB formalism derived in chapter 4, and work done in chapter 7 on the vortex precessional frequencies for triangular and hexagonal vortex arrays and the time-dependent simulations was published in Physical Review A [45].

Chapter 2

Background Theory

2.1 Introduction

In this chapter we consider first the many-body quantum-mechanical problem. A system of identical particles consists of a superposition of all possible permutations of the single-particle wavefunctions. In the case of Bosons, the many-body wavefunction consists of all even permutations of the single-particle wavefunctions, and in the case of Fermions, of all odd permutations. Clearly this is exceedingly complicated. The second quantisation consists of representing the many-body wavefunction in terms of occupation numbers of all possible modes using creation and annihilation operators for each mode. The kets of all possible states consist of occupation numbers for each possible state. These kets span an infinite vector space known as Fock space. The system is characterised by a Hamiltonian represented in terms of these creation and annihilation operators.

The problem in the second quantised form is still formidable, and various approximations need to be made. In this Chapter we consider mean field approximations comprising number-conserving and symmetry-breaking approaches, though most of the emphasis is placed on the Hartree-Fock-Bogoliubov formalism, which is symmetry-breaking. There are other methods only briefly mentioned here, for example, classical field theory which has been successfully applied to higher temperature regimes, and to quasi-condensates, and the truncated Wigner approach.
Chapter 2. Background Theory

2.2 The Many-body Problem

Let us consider a system of $N$ non-relativistic indistinguishable particles confined by some trapping potential $V_T(r_i, t)$ for particle $i$, and let us assume that these particles interact with interaction potential $U(r_i, r_j)$ for two particles $i$ and $j$. The Hamiltonian is then given by

$$\hat{H}(t) = \sum_{i=1}^{N} \hat{h}(r_i, t) + \sum_{i<j} U(r_i, r_j)$$

(2.1)

where

$$\hat{h}(r_i, t) \equiv -\frac{\hbar^2}{2m} \nabla_i^2 + V_T(r_i, t)$$

(2.2)

is the single-particle Hamiltonian for particle $i$. To allow for the indistinguishability of the particles, as will be the case in a quantum gas, we need to take the quantum statistics into account. Generally there are two possibilities for the many-body wave-function, namely symmetric wave-functions (Bosons), and anti-symmetric wave-functions (Fermions). There also exist a third class, called anyons [49], but we shall not be concerned with this here.

In the case of Bosons, the many-body wave-function is symmetric for the exchange of any pair of coordinates, i.e.

$$\Psi^{(S)}(r_1, \ldots, r_i, \ldots, r_j, \ldots, r_N, t) = \Psi^{(S)}(r_1, \ldots, r_j, \ldots, r_i, \ldots, r_N, t)$$

(2.3)

and can be constructed from the summation of all possible permutations of the wave-function with respect to the exchange of coordinates, thus

$$\Psi^{(S)}(r_1, \ldots, r_N, t) = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} \Psi(P \{r_1, \ldots, r_N\}, t)$$

(2.4)

where the symbol $P$ here represents a permutation of the quantities enclosed in curly brackets. Since we can write the many-body wave-function $\Psi(r_1, \ldots, r_N)$ in terms of the individual wave-functions $\psi_{k_i}(r_i, t)$ corresponding to a Boson $i \in \{1, \ldots, N\}$ at $r_i$ in quantum state $k_i$, we obtain [48]

$$\Psi_k^{(S)}(r_1, \ldots, r_N, t) = \frac{1}{\sqrt{N!} \prod_{j} n_j!} \sum_{P \in S_N} P \left\{ \prod_{i=1}^{N} \psi_{k_i}(r_i, t) \right\}$$

(2.5)

for particles $i = 1, \ldots, N$ in states $\{k_i\}$ at positions $\{r_i\}$, where the single particle state $k_i$ appears $n_i$ times in $k = (k_1, \ldots, k_N)$.

In the case of Fermions, the many-body wave-function is anti-symmetric with respect to the exchange of any pair of coordinates, thus

$$\Psi_k^{(A)}(r_1, \ldots, r_i, \ldots, r_j, \ldots, r_N, t) = -\Psi_k^{(A)}(r_1, \ldots, r_j, \ldots, r_i, \ldots, r_N, t)$$

(2.6)
and now we have
\[ \Psi_k^{(A)}(r_1, \ldots, r_N, t) = \frac{1}{\sqrt{N!}} \sum_P (-1)^p P \left\{ \prod_{i=1}^N \psi_k(r_i, t) \right\}. \quad (2.7) \]

Clearly, in the case of Fermions the anti-symmetrised many-body wave-function vanishes when any two particles are in identical states. This leads to a very important principle, the Pauli exclusion principle, and is one of the distinguishing features between Fermions and Bosons. In the case of Bosons, by contrast, the wave-functions are symmetrical. As a consequence of this, it becomes overwhelmingly favourable below a certain transition temperature for the particles to occupy the same quantum state. This is known as Bose-Einstein condensation, and can also be understood in terms of the de Broglie wavelength which, at very low temperature, becomes sufficiently large that the orbitals of all the atoms in the Bose gas overlap. Thus we have, in effect, a single wave-function, and hence all the atoms are coherent. This is analogous to the situation in an optical LASER, thus one can think of a Bose-Einstein Condensate, in the presence of a suitable pumping process, as constituting a matter LASER\(^1\).

We see from the above that such symmetrised and anti-symmetrised many-body wave-functions are highly entangled, therefore we can no longer think of any of the individual particles as being in a particular state \(k_i\), but rather as a superposition of all possible states determined by the many-body wave-function. Solving the many-body quantum-mechanical problem amounts to solving the Schrödinger equation
\[ i\hbar \frac{\partial}{\partial t} \Psi_{k}^{(A,S)}(r_1, \ldots, r_N, t) = \hat{H}(t) \Psi_{k}^{(A,S)}(r_1, \ldots, r_N, t) \quad (2.8) \]

which is clearly intractable except for systems where \(N\) is very small and for a small number of possible states or for some very specific low-dimensional systems in the thermodynamic limit, where exact solutions can be found\(^2\). We can see this since for a system consisting of \(N\) atoms, and restricting the total number of possible states to just \(M\) possible states (in reality there are an infinite number of possible states), there are \(N!\) orderings of the position vectors \(r_i\), and \(M^N\) possible states \(k = (k_1, \ldots, k_N)\). For just 10 atoms and 10 possible states, the number of possible permutations is \(10! \times 10^{10} = 3.63 \times 10^{16}\), hence the number of matrix elements is \((3.63 \times 10^{16})^2 \sim 10^{33}\), which is absolutely prohibitive.

\(^1\)The analogy between an optical LASER and a matter LASER is that we have coherence of the photons in the former case, whereas in the latter case we have coherence of the atoms. It should be noted, however, that there are interactions between the atoms, whereas this is not the case with photons.

\(^2\)There are many well-known examples of exact solutions, see for example [53, 54] for low-dimensional systems having exact solutions in the thermodynamic limit, or [50–52, 130] for exact diagonalisation of the Hamiltonian for very small systems.
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Hence direct solution of the many-body Schrödinger equation (in first quantised form) is impractical except for very small systems, therefore other methods of solution must be found.

2.3 Second-quantization

One can improve the situation by representing the problem (2.8) in terms of mode occupation numbers [48, 55], thus reformulating the problem in terms of quantum field operators. Here we are only concerned with Bosons. We start with equation (2.5)

\[ \Psi_k^{(S)}(r_1, \ldots, r_N, t) = \frac{1}{\sqrt{N!}} \prod_{j=1}^n \frac{1}{n_j!} \sum_{\mathcal{P} \in S_N} \mathcal{P} \left\{ \prod_{i=1}^N \psi_k(r_i, t) \right\} \]

wherein the single particle state \( k \) appears \( n \) times in \( \{k_1, \ldots, k_N\} \). Making use of the result [48]

\[ \int \cdots \int dr_1 \cdots dr_N \Psi_k^{(S)^*} \hat{B}(t) \psi_1^{(S)} = \frac{\sqrt{N!}}{\prod_j n_j!} \int \cdots \int dr_1 \cdots dr_N \Psi_k^{(S)^*} \hat{B}(t) \prod_{i=1}^N \psi_i(r_i, t) \]

(2.9)

for some operator \( \hat{B}(t) \), we obtain

\[ \int \cdots \int dr_1 \cdots dr_N \Psi_k^{(S)^*} \hat{h}(r_i, t) \psi_1^{(S)} = \sum_{\mathcal{P} \in S_N} \mathcal{P} \left\{ \int dr_i \psi_k^{(S)^*} \hat{h}(r_i) \prod_{j \neq i}^N \int dr_j \psi_k^{(S)^*} \psi_j \right\} \]

(2.10)

We note that at least one matrix element vanishes if two or more of the indices in the \( N \)-tuples \( k \) and \( l \) are interchanged, leaving only two options, namely \( k = l \) and the case where \( k \) and \( l \) differ in only one index.

In the first case,

\[ \left\langle \Psi_k^{(S)} \right| \hat{h}(r_i, t) \left| \Psi_k^{(S)} \right\rangle = \left\langle \hat{b}_k \Psi_k^{(S)} \right| n_k \left| \hat{b}^\dagger \Psi_1^{(S)} \right\rangle \left\langle \psi_k \right| \hat{h}(r_i, t) \left| \psi_k \right\rangle \]

since there are \( n_k \) such possibilities, and in the second case

\[ \left\langle \Psi_k^{(S)} \right| \hat{h}(r_i, t) \left| \Psi_l^{(S)} \right\rangle = \left\langle \hat{b}_k \Psi_k^{(S)} \right| \sqrt{n_k n_l} \left| \hat{b}^\dagger \Psi_1^{(S)} \right\rangle \left\langle \psi_k \right| \hat{h}(r_i, t) \left| \psi_l \right\rangle \]

since we now have \( \sqrt{n_k n_l} \) possibilities.

We now establish the exact equivalence of the first (many-body wave-function representation) and second (occupation number representation) quantised forms of the many-body quantum-mechanical problem. In the Dirac notation, this is equivalent to writing
\[ |k\rangle \equiv |k_1 \ldots k_N\rangle \equiv |n_1 \ldots n_j\rangle \]. To establish correspondence with the occupation number representation, we first define the creation and annihilation operators \( \hat{b}_k^\dagger \) and \( \hat{b}_k \) which create and annihilate particles in state \( k \), and write

\[
\begin{align*}
\hat{b}_k^\dagger |n_1 \ldots n_k \ldots \rangle &= \sqrt{n_k + 1} |n_1 \ldots (n_k + 1) \ldots \rangle \\
\hat{b}_k |n_1 \ldots n_k \ldots \rangle &= \sqrt{n_k} |n_1 \ldots (n_k - 1) \ldots \rangle
\end{align*}
\tag{2.11}
\]

hence

\[
\begin{align*}
\hat{b}_k^\dagger \hat{b}_l |n_1 \ldots n_k \ldots \rangle &= \delta_{k,l} n_k |n_1 \ldots n_k \ldots \rangle \\
\hat{b}_k \hat{b}_l^\dagger |n_1 \ldots n_k \ldots \rangle &= \delta_{k,l} (n_k + 1) |n_1 \ldots n_k \ldots \rangle
\end{align*}
\]

so

\[
\left( \hat{b}_k^\dagger \hat{b}_l - \hat{b}_l^\dagger \hat{b}_k \right) |n_1 \ldots n_k \ldots \rangle = \delta_{k,l} |n_1 \ldots n_k \ldots \rangle
\]

Now clearly

\[
\begin{align*}
\left( \hat{b}_k^\dagger \hat{b}_l - \hat{b}_l^\dagger \hat{b}_k \right) |n_1 \ldots n_k \ldots \rangle &= 0 |n_1 \ldots n_k \ldots \rangle \\
\left( \hat{b}_k \hat{b}_l^\dagger - \hat{b}_l \hat{b}_k^\dagger \right) |n_1 \ldots n_k \ldots \rangle &= 0 |n_1 \ldots n_k \ldots \rangle
\]

and therefore we have the Bose commutation relations

\[
\left[ \hat{b}_k, \hat{b}_l^\dagger \right] = \hat{b}_k \hat{b}_l^\dagger - \hat{b}_l^\dagger \hat{b}_k = \delta_{k,l} , \quad \left[ \hat{b}_k, \hat{b}_l \right] = \left[ \hat{b}_k^\dagger, \hat{b}_l^\dagger \right] = 0.
\tag{2.12}
\]

We see from (2.11) that \( \hat{b}_k \Psi_k^{(S)} \rangle \) reduces the occurrence of state \( k_j \) by one with normalisation factor \( \sqrt{n_{kj}} \), hence

\[
\left\langle \Psi_k^{(S)} | \hat{b}_l^\dagger \hat{b}_l \Psi_1^{(S)} \right\rangle = \left\langle \hat{b}_k \Psi_k^{(S)} | \sqrt{n_k n_l} \right\rangle \hat{b}_l \Psi_1^{(S)} \right\rangle
\]

thus establishing the result

\[
\left\langle \Psi_k^{(S)} | \hat{h}(\mathbf{r}_i, t) \Psi_1^{(S)} \right\rangle \equiv h_i(t) \left\langle \Psi_k^{(S)} \right| \hat{b}_l^\dagger \hat{b}_l \right\rangle \Psi_1^{(S)} \right\rangle
\]

where the \( h_i(t) \) are the matrix elements of the single particle Hamiltonian \( \hat{h}(\mathbf{r}_i, t) \) given by

\[
h_i(t) \equiv \langle \psi_i | \hat{h}(\mathbf{r}_i, t) | \psi_i \rangle
\]

Similarly

\[
\left\langle \Psi_k^{(S)} \Psi_1^{(S)} | U(\mathbf{r}_i, \mathbf{r}_j, t) \Psi_m^{(S)} \Psi_n^{(S)} \right\rangle \equiv U_{ij}(t) \left\langle \Psi_k^{(S)} \Psi_1^{(S)} \right| \hat{b}_l^\dagger \hat{b}_l \hat{b}_m \hat{b}_m \right\rangle \Psi_m^{(S)} \Psi_n^{(S)} \right\rangle
\]

with \( U_{ij}(t) \) the matrix elements of the two-body interactions \( U(\mathbf{r}_i, \mathbf{r}_j, t) \) given by

\[
U_{ij}(t) \equiv \langle \psi_k | U(\mathbf{r}_i, \mathbf{r}_j, t) | \psi_i \rangle
\]
Hence we have established the correspondences\(^3\)

\[
\sum_{i=1}^{N} \hat{h}(\mathbf{r}_i, t) \equiv \sum_{k,l=1}^{\infty} \langle k | \hat{h} | l \rangle \hat{b}^\dagger_k \hat{b}_l 
\]

(2.13)

\[
\sum_{i<j}^{N} U(\mathbf{r}_i, \mathbf{r}_j, t) \equiv \frac{1}{2} \sum_{k,l,m,n=1}^{\infty} \langle kl | U | mn \rangle \hat{b}^\dagger_k \hat{b}^\dagger_l \hat{b}_m \hat{b}_n 
\]

(2.14)

thus yielding the Hamiltonian (2.1) in the second quantised form

\[
\hat{H}(t) = \sum_{k,l=1}^{\infty} \langle k | \hat{h} | l \rangle \hat{b}^\dagger_k \hat{b}_l + \frac{1}{2} \sum_{k,l,m,n=1}^{\infty} \langle kl | U | mn \rangle \hat{b}^\dagger_k \hat{b}^\dagger_l \hat{b}_m \hat{b}_n 
\]

(2.15)

Direct solution of the many-body problem in the second-quantised form is still prohibitive, but as we shall see presently, allows us to make certain approximations which make the problem tractable.

### 2.4 Bose Hamiltonian

Let us consider a dilute gas composed of Bosons having interaction potential \(U(\mathbf{r} - \mathbf{r}')\). From a quantum field theoretic viewpoint (see above), we may describe the Boson gas in second quantised form in terms of bosonic creation and annihilation operators. Defining the Bose field operator

\[
\hat{\psi}(\mathbf{r}, t) \equiv \sum_{k=1}^{\infty} \psi_k(\mathbf{r}, t) \hat{b}_k 
\]

(2.16)

and its Hermitian conjugate

\[
\hat{\psi}^\dagger(\mathbf{r}, t) \equiv \sum_{k=1}^{\infty} \psi^*_k(\mathbf{r}, t) \hat{b}^\dagger_k 
\]

(2.17)

we obtain the Bose Hamiltonian in the second quantised form in terms of the Bose field operator \(\hat{\psi}(\mathbf{r}, t)\)

\[
\hat{H}(t) = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}, t) \hat{h}(\mathbf{r}) \hat{\psi}(\mathbf{r}, t) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r'} \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}', t) U(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}', t) \hat{\psi}(\mathbf{r}, t) 
\]

(2.18)

where \(\hat{\psi}^\dagger(\mathbf{r}, t)\) and \(\hat{\psi}(\mathbf{r}, t)\) are creation and annihilation operators corresponding to a Bose field. \(\hat{\psi}^\dagger(\mathbf{r}, t)\) creates a Boson at position \(\mathbf{r}\) while \(\hat{\psi}(\mathbf{r}, t)\) annihilates a Boson at point \(\mathbf{r}\).

\(^3\)The factor \(\frac{1}{2}\) is necessary in order to prevent double counting (hence the summation subscript \(i < j\) on the left hand side of (2.14)).
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	his Hamiltonian we have considered only two-body interactions. The field operator \( \hat{\psi}(\mathbf{r}, t) \) satisfies the usual Bose commutation relations

\[
\left[ \hat{\psi}(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t) \right] = \delta(\mathbf{r} - \mathbf{r}') \quad \text{and} \quad \left[ \hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t) \right] = \left[ \hat{\psi}^\dagger(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t) \right] = 0 \quad (2.19)
\]

and hence the single particle wave-functions \( \{ \psi_k(\mathbf{r}, t) \} \) satisfy the normalisation condition

\[
\sum_k \psi_k(\mathbf{r}, t) \psi_k^*(\mathbf{r}', t) = \delta(\mathbf{r} - \mathbf{r}') \tag{2.20}
\]

by the commutation relations (2.12) for the creation and annihilation operators \( \hat{b}_k^\dagger \) and \( \hat{b}_k \). Since the single particle wave-functions \( \{ \psi_k(\mathbf{r}, t) \} \) form an orthonormal basis, they also satisfy the normalisation condition

\[
\int d\mathbf{r} \psi_k(\mathbf{r}, t) \psi_k^*(\mathbf{r}, t) = \delta_{k,l}. \tag{2.21}
\]

The normalisation conditions (2.20) and (2.21) follow since the \( \{ \psi_k(\mathbf{r}, t) \} \) form a complete orthonormal basis. Equation (2.20) implies that a particle may be found in any one of the states \( \{ \psi_k(\mathbf{r}, t) \} \), which implies completeness. Equation (2.21), on the other hand, implies orthonormality of the basis \( \{ \psi_k(\mathbf{r}, t) \} \). Here \( \hat{h}(\mathbf{r}) \) is the single particle Hamiltonian corresponding to the non-relativistic Schrödinger equation for a single Boson given by

\[
\hat{h}(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V_T(\mathbf{r}) \tag{2.22}
\]

and \( V_T(\mathbf{r}) \) is the trapping potential of the Bose gas. In view of the extremely low energy scales, we may approximate the two-body interaction potential by \( U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}') \) where \( g \) is a coupling constant given in terms of the s-wave scattering length \( a_s \) by the expression

\[
g = \frac{4\pi\hbar^2 a_s}{m}. \tag{2.23}
\]

The s-wave scattering length is obtained by considering a soft pseudo-potential approximation to the two-body interaction potential, and considering only the lowest order scattering processes in the interaction, i.e. s-wave scattering [7, 8]. This is applicable here in view of the extremely low temperatures associated with BECs. The Hamiltonian then becomes

\[
\hat{H}(t) = \int d\mathbf{r} \left( \hat{\psi}^\dagger(\mathbf{r}, t) \hat{h}(\mathbf{r}) \hat{\psi}(\mathbf{r}, t) + \frac{g}{2} \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \right). \tag{2.24}
\]

In the frame rotating with angular frequency \( \Omega \) the single Bose Hamiltonian is given by

\[
\hat{h}_\Omega(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + i\hbar \Omega \cdot (\mathbf{r} \times \nabla) + V_T(\mathbf{r}). \tag{2.25}
\]
Likewise we can write the expression

\[ \hat{h}_v(r) = -\frac{\hbar^2}{2m} \nabla^2 + i\hbar \mathbf{v} \cdot \nabla + V_T(r) \]  \hspace{1cm} (2.26)

for the single Boson Hamiltonian in the frame moving with translational velocity \( \mathbf{v} \).

The problem posed by the Bose Hamiltonian is a formidable one. One could in principle solve the full quantum mechanical problem by solving the Heisenberg equation [7]

\[ i\hbar \frac{\partial}{\partial t} \hat{\psi}(r, t) = \left[ \hat{\psi}(r, t), \hat{H}(t) \right] = \hat{h}(r)\hat{\psi}(r, t) + g\hat{\psi}^\dagger(r, t)\hat{\psi}(r, t)\hat{\psi}(r, t) \]  \hspace{1cm} (2.27)

which describes the dynamics of the Bose field operator \( \hat{\psi}(r, t) \). However, since the Fock space is infinite, we need to restrict the number of possible states by imposing a suitable energy cut-off. The problem is still formidable, however, even for a modest number of atoms, and of possible states. Therefore approximations are necessary. We shall discuss here, various approaches which might be employed to solve the quantum mechanical problem given by the Bose hamiltonian (2.24). Possible approaches include mean-field theories, where we split the Bose field operator \( \hat{\psi}(r, t) \) into a condensate part \( \hat{\Phi}(r, t) \) corresponding to the macroscopically occupied state, and a fluctuation operator part \( \hat{\eta}(r, t) \) corresponding to the non-condensate (thermal) atoms, i.e. \( \hat{\psi}(r, t) = \hat{\Phi}(r, t) + \hat{\eta}(r, t) \), classical field theories wherein we break the Bose field into a condensate band (which we mention only briefly), the truncated Wigner method (which we briefly outline), and path integral methods (not discussed). In the case of the truncated Wigner method, the number of modes used to represent the Bose field determines the size of the computational problem. In practice this number needs to be very large for appreciable propagation times, but the problem is quite practical on a modern desk-top computer. The computational effort required in the HFB approach is determined by the number of computational modes for the condensate wave-function, and the quasi-particle amplitudes, and by the number of modes required for the thermal states to satisfy the required energy cut-off criterion. In practice the number of modes is less than that used by the truncated Wigner method, but the HFB equations need to be solved self-consistently, which can be quite computationally intensive. However this is also quite feasible on modern desk-top computers.

Before discussing these methods, let us comment briefly on the interaction potential, the two-body T-matrix, and the contact potential approximation (which is the approximation used here). \(^4\)

\(^4\)A very good survey of these methods and on the two-body T-matrix may be found in the review article by N. P. Proukakis and B. Jackson [5].
2.5 The Interaction Potential, and the Two-body T-Matrix

The regime of interest here concerns dilute Bose gases at very low temperature. In such a regime, the mean separation between atoms is very large compared with the range of the interatomic potential, hence the effect of short-range interactions are negligible, and may therefore be neglected. So we may describe the atomic interactions in terms of scattering processes, since one is only interested in the effect that the full potential has in the asymptotic limit. In this limit the net effect of the atomic interactions is to bring about a phase shift in the wave-functions of the out-going atoms. Since we are dealing only with very low energies here, only the s-wave scattering processes will be important. In this case one is justified in replacing the interatomic potential \( U(r' - r'') = U(r) \) by a pseudopotential of the form \( U(r) \approx g\delta(r)\partial/\partial r \) [18].

However, this does not take into account the repeated virtual collisions (and thus the repeated action of the interatomic potential \( U(r) \) that might occur during the collision process between two atoms (see figure 2.1). Summation of all Feynmann diagrams gives the Lippmann-Schwinger equation [56]

\[
T_{2b}(z) = U(r) + U(r) \frac{1}{z - \hat{h}(r, t)} T_{2b}(z) \tag{2.28}
\]

for the two-body T-matrix \( T_{2b}(z) \) where \( \hat{h}(r, t) \) is the single-particle Hamiltonian defined earlier with eigenstates \( \{ |k\rangle \} \) and eigenvalues \( \{ \epsilon_k^{SP} \} \). In the representation of the basis of the (complete) set of single particle states \( \{ |k\rangle \} \), we have (see also [23, 24]).

\[
T_{2b}(z) = U(r) + U(r) |kl\rangle \frac{1}{z - \left( \epsilon_k^{SP} + \epsilon_l^{SP} \right)} (kl| T_{2b}(z) \tag{2.29}
\]
and we would replace the bare atomic potential $U(r)$ with the effective interaction potential given by the two-body T-matrix $T_{2b}(z)$.

The contact potential approximation $U(r) \to g\delta(r)$ would amount to replacing the two-body T-matrix $T_{2b}(z)$ by the lowest-order approximation $g\delta(r)$. As we shall see later, making the contact potential approximation leads to ultra-violet (UV) divergences in the anomalous density (defined by equation (2.60)), which is important in mean-field theory beyond the GPE approximation and in perturbation theories. Including higher order terms for the T-matrix provides us with a suitable re-normalisation for the anomalous density, and for energy shifts in perturbation theory. Alternatively, one can impose an energy cut-off (thus eliminating higher energies) since the above treatment is valid only for low energies. The problem here is that the results would depend on this cut-off. However, if this cut-off is chosen judiciously, the errors in this analysis are expected to be relatively small, hence this should not affect qualitatively the conclusions reached concerning the precessional frequencies of vortices in harmonically trapped BECs, for example.

2.6 Mean Field Theories

We discuss two types of mean field theory here, namely symmetry-breaking mean-field theories, and number-conserving mean-field theories.

2.6.1 Symmetry-breaking Mean field Theories

In symmetry-breaking theories, we replace the condensate operator $\hat{\Phi}(r, t)$ in the expression $\hat{\psi}(r, t) = \hat{\Phi}(r, t) + \hat{\eta}(r, t)$ with a c-field (i.e. we regard the condensate operator as a classical field), thus

$$\hat{\psi}(r, t) = \Phi(r, t) + \eta(r, t) \quad (2.30)$$

This is motivated by noting that the number of condensate atoms is given by $\hat{N}_c |N_c\rangle = \int d\mathbf{r} \hat{\Phi}^{\dagger}(r, t) \hat{\Phi}(r, t) |N_c\rangle = N_c |N_c\rangle$, and since

$$\left[ \hat{\Phi}(r, t), \hat{\Phi}^{\dagger}(r', t) \right] = \delta(r - r') \quad (2.31)$$

we find that $\int d\mathbf{r} \hat{\Phi}(r, t) \hat{\Phi}^{\dagger}(r, t) |N_c\rangle = (N_c + 1) |N_c\rangle \approx N_c |N_c\rangle$ for large $N_c$, so for $N_c \to \infty$, we can regard $\hat{\Phi}(r, t)$ and $\hat{\Phi}^{\dagger}(r, t)$ as commuting, and hence we can regard $\Phi(r, t)$ as a classical field $\Phi(r, t)$ in the thermodynamic limit. For a finite system, however, particle
conservation violated. This can also be seen in the light of the breaking of $U(1)$ symmetry. The ansatz $\hat{\psi}(r, t) = \Phi(r, t) + \eta(r, t)$ fixes the phase of the condensate. Since the total number of particles and the global phase are canonically conjugate, this leads to a violation of particle number conservation.

We can, however, fix the number of particles if we work in the Grand-Canonical Ensemble, though this does lead to other issues, for example, the Grand-Canonical catastrophe [12,13] (discussed later at the start of section 2.7). We thus obtain the following second-quantised Grand-Canonical Hamiltonian [11]

$$\hat{H}^{(GC)}(t) = \int d\mathbf{r} \hat{\psi}^\dagger(r, t) \left( \hat{h}(r) - \mu \right) \hat{\psi}(r, t) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{\psi}^\dagger(r, t) \hat{\psi}^\dagger(r', t) U(r-r') \hat{\psi}(r', t) \hat{\psi}(r, t)$$

(2.32)

The Heisenberg equation of motion in the contact potential approximation is then given by

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(r, t) = \left[ \hat{\psi}(r, t), \hat{H}(t) \right] = \left( \hat{h}(r) - \mu \right) \hat{\psi}(r, t) + g \hat{\psi}^\dagger(r, t) \hat{\psi}(r, t) \hat{\psi}(r, t)$$

(2.33)

The inclusion of $\mu$, the chemical potential, ensures that the total number of particles in the system is fixed. Substituting the ansatz $\hat{\psi}(r, t) = \Phi(r, t) + \eta(r, t)$ into the Grand-Canonical Bose Hamiltonian (2.32), we find in the contact potential approximation that

$$\hat{H}^{(GC)}(t) = \hat{H}_0^{(GC)}(t) + \hat{H}_1^{(GC)}(t) + \hat{H}_2^{(GC)}(t) + \hat{H}_3^{(GC)}(t) + \hat{H}_4^{(GC)}(t)$$

(2.34)

where

$$\hat{H}_0^{(GC)}(t) = \int d\mathbf{r} \Phi^* \left( \hat{h} - \mu + \frac{\mathbf{g}}{2} |\Phi|^2 \right) \Phi$$

$$\hat{H}_1^{(GC)}(t) = \int d\mathbf{r} \left( \hat{\eta}^\dagger \left( \hat{h} - \mu + g |\Phi|^2 \right) \Phi + \Phi^* \left( \hat{h} - \mu + g |\Phi|^2 \right) \hat{\eta} \right)$$

$$\hat{H}_2^{(GC)}(t) = \int d\mathbf{r} \left( \hat{\eta}^\dagger \left( \hat{h} - \mu + 2g |\Phi|^2 \right) \hat{\eta} + \frac{\mathbf{g}}{2} \left( \Phi^2 \hat{\eta}^\dagger \hat{\eta} + \Phi^* \hat{\eta}^\dagger \hat{\eta} \right) \right)$$

$$\hat{H}_3^{(GC)}(t) = g \int d\mathbf{r} \left( \Phi \hat{\eta}^\dagger \hat{\eta} + \Phi^* \hat{\eta}^\dagger \hat{\eta} \right)$$

$$\hat{H}_4^{(GC)}(t) = \frac{\mathbf{g}}{2} \int d\mathbf{r} \hat{\eta}^\dagger \hat{\eta}^\dagger \hat{\eta} \hat{\eta}.$$  

The Gross-Pitaevskii Equation

To zeroth order in $\eta$ we can write [5–9]

$$i\hbar \frac{\partial}{\partial t} \Phi(r, t) = \delta \frac{H_0}{\delta \Phi^*} = \left( \hat{h} - \mu + g |\Phi(r, t)|^2 \right) \Phi(r, t).$$

(2.36)

This is the time-dependent Gross-Pitaevskii equation (GPE), and since we have neglected the fluctuation operator completely, this equation is only valid at zero temperature (though
it still neglects vacuum fluctuations at zero temperature). In spite of this, the GPE is still very useful in many situations, and successfully yields the essential behaviour for Bose-Einstein condensates (BECs) in many situations - for example, the precession of vortices [36–40, 79–83], the interference of two condensates [47], etc. The application of the GPE has thus formed an industry in the field.

The Bogoliubov Approximation

One can apply linear response theory to the GPE [6–10] in order to determine the excitation energies of the BEC at \( T \approx 0 \). Writing

\[
\Phi(r, t) = e^{-i\Delta \mu t/\hbar} \left( \phi(r) + e^{-i\epsilon t/\hbar} u(r) + e^{i\epsilon t/\hbar} v^*(r) \right)
\]  

(2.37)

where \( \Delta \mu \) is a shift in the chemical potential determined by the number of condensate atoms given by the Bose-Einstein distribution (2.41), and retaining only terms to first order in \( u(r) \) and \( v(r) \), and equating phase terms \( e^{-i\Delta \mu t/\hbar} \), \( e^{-i(\Delta \mu - \epsilon) t/\hbar} \) and \( e^{-i(\Delta \mu + \epsilon) t/\hbar} \), we obtain the time-independent GPE

\[
\Delta \mu \Phi(r) = \left( \hat{h}(r) - \mu + g |\Phi(r)|^2 \right) \Phi(r)
\]  

(2.38)

and the time-independent Bogoliubov de Gennes Equations (BdGEs)

\[
\epsilon \begin{bmatrix} u(r) \\ v(r) \end{bmatrix} = \begin{bmatrix} \hat{L}_0(r) & \mathcal{M}_0(r) \\ -\mathcal{M}_0^*(r) & -\hat{L}_0^*(r) \end{bmatrix} \begin{bmatrix} u(r) \\ v(r) \end{bmatrix}
\]  

(2.39)

\[
\hat{L}_0(r) \equiv \hat{h}(r) - \mu + 2g |\Phi(r)|^2
\]

\[
\mathcal{M}_0(r) \equiv g\Phi^2(r).
\]  

(2.40)

Here the number of condensate atoms \( N_c \) is given by the Bose-Einstein distribution

\[
N_c = \frac{1}{\exp(\beta \Delta \mu) - 1}
\]  

(2.41)

and in the thermodynamic limit \( \Delta \mu \to 0 \). Here \( \beta \equiv 1/k_B T \) is the temperature parameter, with \( k_B \) the Boltzmann constant and \( T \) the temperature in degrees Kelvin. In the regime of interest (low temperatures, and macroscopic occupation of the ground state), \( \Delta \mu \) is negligible, and can be ignored (see later), thus yielding the usual form for the time-independent GPE

\[
\mu \Phi(r) = \left( \hat{h}(r) + g |\Phi(r)|^2 \right) \Phi(r).
\]  

(2.42)

The energy eigenvalues correspond to the collective excitation energies in the zero-temperature limit (neglecting the thermal density), i.e. at \( T \approx 0 \). This approximation is known as the Bogoliubov approximation [10].
We can also derive the BdGEs in the Bogoliubov approximation from the Heisenberg equation of motion (2.27) by applying the Bogoliubov transformation

$$\hat{\eta}(\mathbf{r}, t) = \sum_k \left( u_k(\mathbf{r}, t) \hat{a}_k + v_k^*(\mathbf{r}, t) \hat{a}_k^\dagger \right)$$

for the fluctuation operator $\hat{\eta}(\mathbf{r}, t)$, with Hermitian conjugate

$$\hat{\eta}^\dagger(\mathbf{r}, t) = \sum_k \left( v_k(\mathbf{r}, t) \hat{a}_k + u_k^*(\mathbf{r}, t) \hat{a}_k^\dagger \right).$$

Here we have expanded the fluctuation operator $\hat{\eta}(\mathbf{r}, t)$ in a weakly-interacting quasi-particle basis. The assumption here is that the quasi-particles are non-interacting. The operators $\hat{a}_k^\dagger$ and $\hat{a}_k$ are creation and annihilation operators for these quasi-particles, and the $u_k(\mathbf{r}, t)$ and $v_k^*(\mathbf{r}, t)$ are the associated quasi-particle amplitudes. This transformation is canonical, hence the Bose commutation relations are preserved, i.e.

$$\left[ \hat{a}_k, \hat{a}_l^\dagger \right] = \delta_{k,l} \text{ and } \left[ \hat{a}_k, \hat{a}_l \right] = \left[ \hat{a}_k^\dagger, \hat{a}_l^\dagger \right] = 0.$$  

The creation and annihilation operators $\hat{a}_k^\dagger$ and $\hat{a}_k$ are given in terms of the fluctuation operator $\hat{\eta}(\mathbf{r}, t)$, and the quasi-particle amplitudes $u_k(\mathbf{r}, t)$ and $v_k^*(\mathbf{r}, t)$ by the inverse Bogoliubov transformation

$$\hat{a}_k = \int d\mathbf{r} \left( u_k^*(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) - v_k^*(\mathbf{r}, t) \hat{\eta}^\dagger(\mathbf{r}, t) \right)$$

with Hermitian conjugate

$$\hat{a}_k^\dagger = \int d\mathbf{r} \left( -v_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) + u_k(\mathbf{r}, t) \hat{\eta}^\dagger(\mathbf{r}, t) \right).$$

Then, using the commutation relations

$$\left[ \hat{\psi}(\mathbf{r}, t), \hat{a}_k^\dagger \right] = u_q(\mathbf{r}, t), \quad \left[ \hat{\psi}(\mathbf{r}, t), \hat{a}_k \right] = v_q^*(\mathbf{r}, t), \quad \left[ \hat{\psi}^\dagger(\mathbf{r}, t), \hat{a}_k^\dagger \right] = v_q(\mathbf{r}, t), \quad \left[ \hat{\psi}^\dagger(\mathbf{r}, t), \hat{a}_k \right] = u_q^*(\mathbf{r}, t),$$

we find to first order in $\hat{\eta}(\mathbf{r}, t)$

$$i\hbar \frac{\partial u_q(\mathbf{r}, t)}{\partial t} = \left( \hat{\Phi}(\mathbf{r}) - \mu + 2g|\Phi(\mathbf{r}, t)|^2 \right) u_q(\mathbf{r}, t) + g\Phi^2(\mathbf{r}, t) v_q(\mathbf{r}, t)$$

and

$$i\hbar \frac{\partial v_q^*(\mathbf{r}, t)}{\partial t} = \left( \hat{\Phi}(\mathbf{r}) - \mu + 2g|\Phi(\mathbf{r}, t)|^2 \right) v_q^*(\mathbf{r}, t) + g\Phi^2(\mathbf{r}, t) u_q^*(\mathbf{r}, t)$$

which yields the BdGEs

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(\mathbf{r}, t) \\ v_q(\mathbf{r}, t) \end{bmatrix} = \begin{bmatrix} \hat{L}_0(\mathbf{r}, t) & \hat{M}_0(\mathbf{r}, t) \\ -\hat{M}_0^*(\mathbf{r}, t) & -\hat{L}_0^*(\mathbf{r}, t) \end{bmatrix} \begin{bmatrix} u_q(\mathbf{r}, t) \\ v_q(\mathbf{r}, t) \end{bmatrix}$$
in the Bogoliubov approximation.

The corresponding time-independent BdGEs are

\[
\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \begin{bmatrix} \hat{\mathcal{L}}_0(r) & \mathcal{M}_0(r) \\ -\mathcal{M}_0^*(r) & -\hat{\mathcal{L}}_0^*(r) \end{bmatrix} \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix}.
\] (2.50)

The quasi-particle occupation numbers are given by the Bose distribution

\[
N_{BE}(\epsilon_q) = \frac{1}{\exp(\beta \epsilon_q) - 1},
\] (2.51)

hence one can calculate the mean thermal density

\[
\bar{n}(r, t) = \langle \hat{n}^\dagger(r, t) \hat{n}(r, t) \rangle = \sum_q |u_q(r, t)|^2 N_{BE}(\epsilon_q) + |v_q(r, t)|^2 (N_{BE}(\epsilon_q) + 1).
\] (2.52)

Since the Bogoliubov transformation is canonical, and hence the commutation relations (2.45) hold, the following orthogonality and symmetry relations for the quasi-particle amplitudes

\[
\int dt \, (u^*_k(r, t) u_l(r, t) - v^*_k(r, t) v_l(r, t)) = \delta_{k,l}
\]

\[
\int dt \, (u^*_k(r, t) v_l(r, t) - v^*_k(r, t) u_l(r, t)) = 0
\] (2.53)

\[
\int dt \, (u_k(r, t) v_l(r, t) - v_k(r, t) u_l(r, t)) = 0
\]

must also hold, thus establishing the normalisation condition

\[
\int dr \, (|u_k(r, t)|^2 - |v_k(r, t)|^2) = 1
\] (2.54)

for the quasi-particle amplitudes.

The linear response treatment demonstrates, in the presence of a condensate, the equivalence of the collective modes and the quasi-particle excitations. We therefore associate the Bogoliubov energy spectrum with the collective excitations at \( T = 0 \).

**The Hartree-Fock-Bogoliubov (HFB) Equations**

We can use the factorisation approximations [11]

\[
\hat{n}^\dagger(r, t) \hat{n}(r, t) \approx 2\bar{n}(r, t) \hat{n}(r, t) + \bar{m}(r, t) \hat{n}^\dagger(r, t)
\]

\[
\hat{n}^\dagger(r, t) \hat{n}^\dagger(r, t) \hat{n}(r, t) \approx 2\bar{n}(r, t) \hat{n}^\dagger(r, t) + \bar{m}^*(r, t) \hat{n}(r, t)
\]

\[
\hat{n}^\dagger(r, t) \hat{n}^\dagger(r, t) \hat{n}(r, t) \hat{n}(r, t) \approx 4\bar{n}(r, t) \hat{n}^\dagger(r, t) \hat{n}(r, t) + \bar{m}(r, t) \hat{n}^\dagger(r, t) \hat{n}^\dagger(r, t) \hat{n}(r, t)
\]

\[
+ \bar{m}^*(r, t) \hat{n}(r, t) \hat{n}(r, t) - 2\bar{n}^2(r, t) - |\bar{m}(r, t)|^2
\] (2.55)

\[
\hat{H}^{(GC)}(t) \approx \hat{H}_{HFB}(t)
\] (2.56)
where we define the HFB Hamiltonian
\[ \hat{H}_{HFB}(t) \equiv \hat{H}_{HFB_0}(t) + \hat{H}_{HFB_1}(t) + \hat{H}_{HFB_2}(t). \] (2.57)

In the expression (2.57) for the Hamiltonian, we have broken the HFB Hamiltonian into Hamiltonians of zeroth, first and second order in terms of the annihilation and creation fluctuation operators \( \hat{\eta} \) and \( \hat{\eta}^\dagger \), viz.
\[
\begin{align*}
\hat{H}_{HFB_0}(t) & \equiv \int \, d\mathbf{r} \left( \Phi^* \left( \hat{h} - \mu + \frac{g}{2} |\Phi|^2 \right) \Phi - g \left( \tilde{n}^2 + \frac{1}{2} |\tilde{m}|^2 \right) \right) \\
\hat{H}_{HFB_1}(t) & \equiv \int \, d\mathbf{r} \left( \hat{\eta}^\dagger \left( \hat{h} - \mu \right) \Phi + \Phi^* \left( \hat{h} - \mu \right) \hat{\eta} + g \left[ \left( |\Phi|^2 + 2\tilde{n} \right) \Phi^* + \tilde{m}^* \Phi \right] \hat{\eta} + \text{h.c.} \right) \\
\hat{H}_{HFB_2}(t) & \equiv \int \, d\mathbf{r} \left( \hat{\eta}^\dagger \left( \hat{h} - \mu \right) \hat{\eta} + \frac{g}{2} \left( \Phi^* \Phi + \tilde{m}^* \tilde{m} \right) \hat{\eta} \hat{\eta} + (\Phi^2 + \tilde{m}) \hat{\eta}^\dagger \hat{\eta}^\dagger + 4 \left( |\Phi|^2 + \tilde{n} \right) \hat{\eta}^\dagger \hat{\eta} \right)
\end{align*}
\] (2.58)

and where we have defined the thermal density as before (2.52)
\[
\tilde{n}(\mathbf{r}, t) \equiv \langle \hat{\eta}^\dagger(\mathbf{r}, t)\hat{\eta}(\mathbf{r}, t) \rangle = \sum_q \left[ |u_q(\mathbf{r}, t)|^2 N_{BE}(\epsilon_q) + |v_q(\mathbf{r}, t)|^2 (N_{BE}(\epsilon_q) + 1) \right] \tag{2.59}
\]

and the anomalous density
\[
\tilde{m}(\mathbf{r}, t) \equiv \langle \hat{\eta}(\mathbf{r}, t)\hat{\eta}(\mathbf{r}, t) \rangle = \sum_q u_q(\mathbf{r}, t)v_q^*(\mathbf{r}, t) (2N_{BE}(\epsilon_q) + 1) \tag{2.60}
\]

with the Bose distribution for the \( q^{th} \) quasi-particle excitation \( N_{BE}(\epsilon_q) \) given by (2.51)
\[
N_{BE}(\epsilon_q) = \frac{1}{\exp(\beta \epsilon_q) - 1}.
\]

We then make use of the Heisenberg equation of motion (2.27). We can derive the generalised Gross-Pitaevskii equation (GGPE) from the Heisenberg equation for the ensemble-averaged quantity \( \langle \hat{\psi}(\mathbf{r}, t) \rangle \)
\[
\begin{align*}
\imath \hbar \frac{\partial}{\partial t} \langle \hat{\psi}(\mathbf{r}, t) \rangle = & \left[ \hat{\psi}(\mathbf{r}, t), \hat{\mathcal{H}}(t) \right] = \langle \left( \hat{\mathcal{H}}(\mathbf{r}) - \mu \right) \hat{\psi}(\mathbf{r}, t) \rangle + g \langle \hat{\psi}^\dagger(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t) \rangle.
\end{align*}
\]

We expand the expression \( \langle \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \rangle \) in terms of the Bogoliubov shift \( \hat{\psi} = \Phi + \hat{\eta} \). We note that \( \Phi = \langle \hat{\psi} \rangle \), and apply Wick’s theorem for ensemble averages to the operator pairs \( \langle \hat{\eta}^\dagger \hat{\eta} \rangle \) and \( \langle \hat{\eta} \hat{\eta} \rangle \). Thus we obtain the self-consistent mean-field approximation [11]
\[
\begin{align*}
\langle \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \rangle = & \left( |\Phi|^2 + 2\tilde{n} \right) \Phi + \tilde{m} \Phi^*, \quad \text{where} \quad \tilde{n} \equiv \langle \hat{\eta}^\dagger \hat{\eta} \rangle, \quad \text{and} \quad \tilde{m} \equiv \langle \hat{\eta} \hat{\eta} \rangle.
\end{align*}
\]

Hence we obtain the generalised Gross-Pitaevskii equation (2.62). Applying the commutation relations (2.48) to the Heisenberg equation of motion (2.33), we have in the mean field approximation
\[
\begin{align*}
\imath \hbar \frac{\partial}{\partial t} u_q(\mathbf{r}, t) = & \left( \hat{\mathcal{H}}(\mathbf{r}) - \mu \right) u_q(\mathbf{r}, t) + 2g \langle \hat{\psi}^\dagger(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t) \rangle u_q(\mathbf{r}, t) + g \langle \hat{\psi}(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t) \rangle v_q(\mathbf{r}, t)
\end{align*}
\]
and since \( \langle \hat{\psi}^\dagger \hat{\psi} \rangle = |\Phi|^2 + \tilde{n} \) and \( \langle \hat{\psi} \hat{\psi}^\dagger \rangle = \Phi^2 + \tilde{m} \), we find that
\[
\frac{i\hbar}{\partial t} u_q(r, t) = \left( \hat{h}(r) - \mu \right) u_q(r, t) + 2g \left( |\Phi(r, t)|^2 + \tilde{n}(r, t) \right) u_q(r, t) + g \left( \Phi^2(r, t) + \tilde{m}(r, t) \right) v_q(r, t).
\]
We can obtain the same result by applying the commutation relations (c.f. Eq. (2.19))
\[
\left[ \hat{\eta}(r, t), \hat{\psi}^\dagger(r', t) \right] = \delta(r - r') \quad \text{and} \quad \left[ \hat{\eta}(r, t), \hat{\psi}(r', t) \right] = \left[ \hat{\psi}^\dagger(r, t), \hat{\psi}^\dagger(r', t) \right] = 0 \quad (2.61)
\]
and the commutation relations (2.48) to the HFB Hamiltonian (2.57). Similarly
\[
\frac{i\hbar}{\partial t} v^*_q(r, t) = \left( \hat{h}(r) - \mu \right) v^*_q(r, t) + 2g \left( |\Phi|^2 + \tilde{n} \right) v^*_q(r, t) + g \left( \Phi^2 + \tilde{m} \right) u^*_q(r, t)
\]
with complex conjugate
\[
-\frac{i\hbar}{\partial t} v_q(r, t) = \left( \hat{h}^*(r) - \mu \right) v_q(r, t) + 2g \left( |\Phi|^2 + \tilde{n} \right) v_q(r, t) + g \left( \Phi^2 + \tilde{m}^* \right) u_q(r, t).
\]
Thus we obtain the time-dependent HFB equations [61] consisting of the generalised Gross-Pitaevskii equation (GGPE)
\[
\frac{i\hbar}{\partial t} \Phi(r, t) = \left( \hat{h}(r) - \mu + g \left( |\Phi(r, t)|^2 + 2\tilde{n}(r, t) \right) \right) \Phi(r, t) + g\tilde{m}(r, t) \Phi^*(r, t) \quad (2.62)
\]
and the Bogoliubov de Gennes equations (BdGEs)
\[
\frac{i\hbar}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \begin{bmatrix} \hat{\mathcal{L}}(r, t) & \mathcal{M}(r, t) \\ -\mathcal{M}^*(r, t) & -\hat{\mathcal{L}}^*(r, t) \end{bmatrix} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} \quad (2.63)
\]
for the quasi-particle amplitudes, where
\[
\hat{\mathcal{L}}(r, t) \equiv \hat{h}(r) - \mu + 2g \left( |\Phi(r, t)|^2 + \tilde{n}(r, t) \right)
\]
\[
\mathcal{M}(r, t) \equiv g \left( \Phi^2(r, t) + \tilde{m}(r, t) \right). \quad (2.64)
\]
The corresponding time-independent equations are given by the time-independent GGPE
\[
\Delta \mu \Phi(r) = \left( \hat{h}(r) - \mu + g \left( |\Phi(r)|^2 + 2\tilde{n}(r) \right) \right) \Phi(r) + g\tilde{m}(r) \Phi^*(r) \quad (2.65)
\]
and the time-independent BdGEs
\[
\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \begin{bmatrix} \hat{\mathcal{L}}(r) & \mathcal{M}(r) \\ -\mathcal{M}^*(r) & -\hat{\mathcal{L}}^*(r) \end{bmatrix} \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} \quad (2.66)
\]
with
\[
\hat{\mathcal{L}}(r) \equiv \hat{h}(r) - \mu + 2g \left( |\Phi(r)|^2 + \tilde{n}(r) \right)
\]
\[
\mathcal{M}(r) \equiv g \left( \Phi^2(r) + \tilde{m}(r) \right). \quad (2.67)
\]
Problems with the Standard HFB Theory  The symmetry-breaking approximation, the mean field approximation, and the admission of a non-interacting quasi-particle basis (where we effectively ignore the quasi-particle interactions) leads to inconsistencies in the treatment of the condensate and non-condensate. This in turn leads to an unphysical gap in the energy spectrum, and also to the violation of the Hugenholtz-Pines theorem [11]. We deal with these problems in turn

1. Gap in Excitation Energy Spectrum - The gap in the excitation energy spectrum is a direct consequence of the above-mentioned inconsistencies. We shall see later in the time-independent perturbation that the energy gap is due to the neglect of the cubic terms $\Phi \hat{\eta}^\dagger \hat{\eta} \hat{\eta}^\dagger$ and $\Phi^* \hat{\eta}^\dagger \hat{\eta} \hat{\eta}^\dagger$ which are omitted in the derivation of the HFB equations by virtue of the fact that $\langle \hat{\eta}^\dagger \hat{\eta} \hat{\eta}^\dagger \rangle = \langle \hat{\eta}^\dagger \hat{\eta} \hat{\eta}^\dagger \rangle = \langle \hat{\eta}^\dagger \rangle = \langle \hat{\eta} \rangle = 0$ for ensemble averages for a non-interacting quasi-particle basis.

2. Violation of the Hugenholtz-Pines Theorem for HFB - The Hugenholtz-Pines theorem [11] requires the existence of a zero-energy quasi-particle state that is proportional to the ground state. We show this is not the case for standard HFB.

To show how the Hugenholtz-Pines theorem is violated, let us write $u_0 = \phi$, $v_0 = -\phi^*$ where $\phi$ is a wave function proportional to the condensate wavefunction $\Phi$, and which is normalised to unity, ie.

$$\int dr |\phi(r)|^2 = 1 \quad (2.68)$$

so, in fact $\phi = \Phi/\sqrt{N_c}$, where $N_c$ is the total number of condensate atoms. Then, substituting $u_0$, $v_0$ into the first of the time-independent BdGEs (2.66), we find that

$$\epsilon_0 \phi = \left(\hat{h} + 2g (|\Phi|^2 + \tilde{n})\right) \phi - g (\tilde{\mu} + \Phi^2) \phi^* = -2g \tilde{m} \phi^* + \Delta \mu \phi \quad (2.69)$$

since $\left(\hat{h} + g (2 |\Phi|^2 + \tilde{n})\right) \phi + g \tilde{m} \phi^* = \Delta \mu \phi$ by the GGPE (2.65). Multiplying both sides by $\phi^*$, and integrating over all space, we find (in view of the orthogonality of $\phi$) that

$$\epsilon_0 = -2g \int dr \phi^* \phi (r) \tilde{m}(r) + \Delta \mu \neq 0 \quad (2.70)$$

so the Goldstone mode does not exist.

The Popov approximation, and the gapless G1 and G2 Theories

The Popov Approximation [11]  The easiest remedy to the above-mentioned problems is simply to ignore the anomalous density. This is known as the Popov approximation,
which we see from equation (2.70), is gapless in the thermodynamic limit. This approximation is not justified by the fact that the anomalous density \(\tilde{m}\) is small (indeed \(\tilde{m}\) is often of the same order as \(\tilde{n}\)), but rather that in order to deal with the interactions between condensate and non-condensate particles in a consistent manner, one needs to proceed beyond the quadratic Hamiltonian approximation. The justification of the Popov approximation [15–17] is that two-body correlations are represented by the anomalous density \(\tilde{m}\), and therefore the s-wave scattering length \(a_s\) is already measured in the presence of two-body collisions (correlations). In order to understand this we need to remember that the contact potential approximation \(U(r - r') = g\delta(r - r')\) where \(g \equiv 4\pi\hbar^2a_s/m\) used here represents an approximation to the 2-body T-matrix, and not to the bare interaction potential \(U(r)\). Therefore including \(\tilde{m}\) means counting these correlations twice. This inconsistency is addressed by ignoring \(\tilde{m}\). However, as we shall see, this results in the violation of particle conservation, and of linear and angular momentum.

We can also address this issue by using the perturbative methods outlined by S. A. Morgan [23, 24] (see section dealing with number-conserving theories 2.7), or alternatively, using the G1 and G2 gapless approximations as will be discussed now.

**The G1 and G2 Gapless Approximations** If one wishes to go beyond the two-body T-matrix, this can be achieved by replacing the contact potential approximation to the interaction potential in the GPE (2.42) and in the BdGEs (2.50) in the Bogoliubov approximation by the expression \(g\left(1 + \frac{\tilde{m}(r)}{\Phi^2(r)}\right)\) thereby introducing the anomalous density into the formalism. It can be shown that this is equivalent to replacing the bare interaction \(U(r - r')\) with the many-body T-matrix in the low momentum limit [15–17, 19, 21]. Consideration of the time-independent GGPE (2.65)

\[
\mu \Phi(r) = \left(\hat{h}(r) + g \left(\Phi^2(r) + 2\tilde{n}(r)\right)\right) \Phi(r) + g\tilde{m}(r)\Phi^*(r)
\]

shows that grouping the term \(\Phi^2\Phi\) with the term \(\tilde{m}\Phi^*\) gives

\[
g \left(1 + \frac{\tilde{m}}{\Phi^2}\right) \Phi^2 \Phi = g \left(1 + \frac{\tilde{m}}{\Phi^2}\right) \Phi^2 \Phi
\]

enabling us to rewrite the GGPE as

\[
\mu \Phi(r) = \left(\hat{h}(r) + U_s(r) \left|\Phi(r)\right|^2 + 2g\tilde{n}(r)\right) \Phi(r)
\]

(2.71)

where

\[
U_s(r) = g \left(1 + \frac{\tilde{m}(r)}{\Phi^2(r)}\right)
\]

(2.72)

is an effective interaction which, as alluded to above, may be shown to be equivalent to the many-body T-matrix in the low-momentum limit. One may then deal with the time-
independent Bogoliubov de Gennes Equations (BdGEs) (2.50)

\[
\epsilon \begin{bmatrix} u(r) \\ v(r) \end{bmatrix} = \begin{bmatrix} \hat{L}_0(r) & \mathcal{M}_0(r) \\ -\mathcal{M}_0^*(r) & -\hat{L}_0^*(r) \end{bmatrix} \begin{bmatrix} u(r) \\ v(r) \end{bmatrix}
\]  

(2.73)

by a similar introduction of the effective interaction which, depending on whether the condensate and non-condensate interactions are treated on the same basis, yields two distinct gapless theories known as the G1 and G2 gapless theories, which are collectively known as the gapless Hartree-Fock Bogoliubov (GHFB) theories. One uses either G1 or G2 depending on the particular temperature regime of interest. In the low-momentum regime, many-body effects are important, and hence we expect the interactions between condensed and excited atoms to be the same as that between two condensed atoms, and we use the effective interactions

\[
U_c(r) = g \left( 1 + \frac{\tilde{m}(r)}{\Phi^2(r)} \right)
\]

and

\[
U_e(r) = g \left( 1 + \frac{\tilde{m}(r)}{\Phi^2(r)} \right)
\]

respectively for the condensed and non-condensed atoms, thus motivating the G2 gapless theory.

The G1 gapless theory, on the other hand, is more applicable in the regime of relatively high momentum (higher \(T\)). Here we would model the condensate interactions using

\[
U_c(r) = g \left( 1 + \frac{\tilde{m}(r)}{\Phi^2(r)} \right),
\]

whereas we would use \(U_e(r) = g\) for the non-condensate interactions.

The Popov, and the gapless G1 and G2 theories may be summarised as follows:

\[
\mu \Phi(r) = \left( \hat{h}(r) + U_c(r) |\Phi(r)|^2 + 2U_e(r)\tilde{n}(r) \right) \Phi(r)
\]

(2.74)

and

\[
\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \begin{bmatrix} \hat{L}_G(r) & \mathcal{M}_G(r) \\ -\mathcal{M}_G^*(r) & -\hat{L}_G^*(r) \end{bmatrix} \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix}
\]

(2.75)

where

\[
\hat{L}_G(r) \equiv \hat{h}(r) - \mu + 2U_c(r) |\Phi(r)|^2 + 2U_e(r)\tilde{n}(r)
\]

\[
\mathcal{M}_G(r) \equiv U_c(r)\Phi^2(r)
\]

(2.76)

with

\[
U_c(r) = g \left( 1 + a \frac{\tilde{m}(r)}{\Phi^2(r)} \right)
\]

(2.77)

and

\[
U_e(r) = g \left( 1 + b \frac{\tilde{m}(r)}{\Phi^2(r)} \right)
\]

(2.78)

where

\[
a = \begin{cases} 
0 & \text{Popov} \\
1 & \text{G1} \\
1 & \text{G2} 
\end{cases}
\]

(2.79)
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and

\[ b = \begin{cases} 
0 & \text{Popov} \\
0 & \text{G1} \\
1 & \text{G2} 
\end{cases} \tag{2.80} \]

for the time-independent Popov, G1 and G2 equations. In the Popov approximation, this reduces to the GGPE

\[ \mu \Phi(r) = \left( \hat{h}(r) + g \left( |\Phi(r)|^2 + 2\tilde{n}(r) \right) \right) \Phi(r) \tag{2.81} \]

and the BdGEs

\[ \epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \begin{bmatrix} \hat{L}_P(r) & \mathcal{M}_P(r) \\ -\mathcal{M}_P(r) & -\hat{L}_P(r) \end{bmatrix} \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} \tag{2.82} \]

where

\[ \hat{L}_P(r) \equiv \hat{h}(r) - \mu + 2g \left( |\Phi(r)|^2 + \tilde{n}(r) \right) \]

\[ \mathcal{M}_P(r) \equiv g\Phi^2(r). \tag{2.83} \]

Since the interactions are now suitably re-normalised, the problem due to the double counting of \( \tilde{m} \) no longer exists, and the GHFB formalisms are gapless. The \( m = 2 \) excitation energy spectrum predicted by GHFB for a dilute Bosonic gas with repulsive interactions in a TOP trap [19] is in close agreement with the JILA experiment [20], and represents a substantial improvement over the Popov prediction. The \( m = 0 \) upward shift in the energy spectrum for \( T \gtrsim T_c / 2 \), however remains unexplained with both GHFB and Popov, which both predict a downward shift. Explanation of these energy shifts requires the inclusion of the thermal cloud dynamics [58–60]. This was done by achieved most convincingly by Morgan et. al. [60] using a linear response analysis on the generalised GPE subject to an external potential \( P(r,t) \) given by

\[ i\hbar \frac{\partial}{\partial t} \Phi(r,t) = \left( \hat{h}(r) + P(r,t) + g \left( |\Phi(r,t)|^2 + 2\tilde{n}(r,t) \right) \right) \Phi(r,t) + g\tilde{n}(r,t)\Phi^*(r,t) - f(r,t) \tag{2.84} \]

with \( f(r,t) \) defined as

\[ f(r,t) = \frac{g}{N_c} \sum_q \left[ c_q^* N_{\text{BE}}(\epsilon_q) u_q(r,t) + c_q (N_{\text{BE}}(\epsilon_q) + 1) v_q^*(r,t) \right] \tag{2.85} \]

where \( N_c \) is the condensate population, and where

\[ c_q(t) = \int d\mathbf{r} |\Phi(\mathbf{r},t)|^2 \left[ \Phi^*(\mathbf{r},t) u_q(\mathbf{r},t) + \Phi(\mathbf{r},t) v_q(\mathbf{r},t) \right]. \tag{2.86} \]
2.6.2 Other Symmetry-breaking Theories

In the HFB formalism, one applies the Bogoliubov transformation (2.43) to express the fluctuation operator \( \hat{\eta}(\mathbf{r}, t) \) in terms of creation and annihilation operators \( \hat{a}^\dagger \) and \( \hat{a}_q \), and amplitudes \( u_q(\mathbf{r}, t) \) and \( v^*_q(\mathbf{r}, t) \) corresponding to these operators, for a system of non-interacting quasi-particles. We choose \( \hat{a}^\dagger \) and \( \hat{a}_q \) to be time-independent, and this allows the dynamics of the non-condensate to be expressed completely in terms of the quasi-particle amplitudes \( u_q(\mathbf{r}, t) \) and \( v^*_q(\mathbf{r}, t) \), which contain all the time-dependence in the evolution of the fluctuation operator \( \hat{\eta}(\mathbf{r}, t) \).

An alternative approach [62–64] is to use the Heisenberg equation of motion to derive a set of equations for the operator pairs \( \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \) and \( \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \) where the position vectors \( \mathbf{r}' \) and \( \mathbf{r}'' \) are independent, thus double integration is implied with respect to \( \mathbf{r}' \) and \( \mathbf{r}'' \) in evaluation of the matrix elements. This is necessary in order to allow pairing of operators with respect to differential operators, thus facilitating taking expectation values when determining the equations of motion for the normal and anomalous generalised correlation densities \( G_N(\mathbf{r}', \mathbf{r}'', t) \equiv \langle \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \rangle \) and \( G_A(\mathbf{r}', \mathbf{r}'', t) \equiv \langle \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \rangle \), and their reverse-ordered Hermitian conjugates \( G^C_N(\mathbf{r}', \mathbf{r}'', t) \equiv \langle \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \rangle \) and \( G^C_A(\mathbf{r}', \mathbf{r}'', t) \equiv \langle \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \rangle \). The dynamical equation for the condensate density \( \Phi(\mathbf{r}, t) \) is given by the GGPE (2.62), whilst the dynamical equations for \( G_N(\mathbf{r}', \mathbf{r}'', t) \) and \( G_A(\mathbf{r}', \mathbf{r}'', t) \) are found by taking the expectation values of the operators in the dynamical equations for \( \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \) and \( \hat{\eta}(\mathbf{r}', t)\hat{\eta}(\mathbf{r}'', t) \), and applying Wick’s theorem for ensemble averages, subject to the assumption of a Hamiltonian that is approximately quadratic. Let us define the density matrix

\[ G(\mathbf{r}', \mathbf{r}'', t) \equiv \begin{bmatrix} G_N(\mathbf{r}', \mathbf{r}'', t) & G_A(\mathbf{r}', \mathbf{r}'', t) \\ G^*_A(\mathbf{r}', \mathbf{r}'', t) & G^C_N(\mathbf{r}', \mathbf{r}'', t) \end{bmatrix} \]  

and the operator matrix

\[ \hat{\mathbf{L}}(\mathbf{r}, t) \equiv \begin{bmatrix} \hat{\mathbf{L}}(\mathbf{r}, t) & \mathbf{M}(\mathbf{r}, t) \\ -\mathbf{M}^*(\mathbf{r}, t) & -\hat{\mathbf{L}}^*(\mathbf{r}, t) \end{bmatrix} \]  

where the operators \( \hat{\mathbf{L}}(\mathbf{r}, t) \) and \( \mathbf{M}(\mathbf{r}, t) \) are defined by

\[ \hat{\mathbf{L}}(\mathbf{r}, t) \equiv \hat{\mathbf{h}}(\mathbf{r}) - \mu + 2g (|\Phi(\mathbf{r}, t)|^2 + G_N(\mathbf{r}, \mathbf{r}, t)) \]  

\[ \mathbf{M}(\mathbf{r}, t) \equiv g (\Phi^2(\mathbf{r}, t) + G_A(\mathbf{r}, \mathbf{r}, t)) \]  

then the dynamical equations for \( G_N(\mathbf{r}', \mathbf{r}'', t) \) and \( G_A(\mathbf{r}', \mathbf{r}'', t) \) and their reverse-ordered Hermitian conjugates may be written in the matrix form [62–64]

\[ i\hbar \frac{\partial}{\partial t} G(\mathbf{r}', \mathbf{r}'', t) = \hat{\mathbf{L}}(\mathbf{r}'', t)G(\mathbf{r}', \mathbf{r}'', t) - G(\mathbf{r}', \mathbf{r}'', t) \hat{\mathbf{L}}^*(\mathbf{r}', t). \]
It should be stressed here that these equations are only valid for $r'$ and $r''$ being independent position vectors, implying double integration in determining the matrix elements. This also implies that there is no simple dynamical equation for the auto-correlation densities, for example the thermal density $\tilde{n}$ and the anomalous density $\tilde{m}$ as in the time-dependent HFB formalism discussed earlier, but one can derive an equation for these quantities in terms of the coefficients of $G_N$ and $G_A$ expanded in the single particle basis, viz.

$$G_N(r',r'',t) = \sum_{kl} G_{Nkl}(t) \xi_k^*(r') \xi_l(r'') \tag{2.91}$$

and

$$G_A(r',r'',t) = \sum_{kl} G_{Akl}(t) \xi_k(r') \xi_l(r''). \tag{2.92}$$

One determines the dynamical equation for the coefficients $G_{Nkl}(t)$ and $G_{Akl}(t)$ of the normal and anomalous densities $G_N(r',r'',t)$ and $G_A(r',r'',t)$ and their respective reverse-ordered Hermitian conjugates by substituting (2.91) and (2.92) into equation (2.90). Multiplying both sides of the resulting equation by $\xi^*_k(r') \xi^*_l(r'')$ and $\xi_k(r') \xi_l(r'')$, and integrating with respect to the position coordinates $r'$ and $r''$ over all space yields the respective dynamical equations for the coefficients $G_{Nkl}(t)$ and $G_{Akl}(t)$ in terms of the relevant matrix products. Then we can write

$$\tilde{n}(r,t) = \sum_{kl} G_{Akl}(t) \xi_k^*(r) \xi_l(r) \tag{2.93}$$

for the thermal density, and

$$\tilde{m}(r,t) = \sum_{kl} G_{Nkl}(t) \xi_k(r) \xi_l(r) \tag{2.94}$$

for the anomalous density. One can use equation (2.93) to attempt to establish a correspondence with the time-dependent HFB formalism described in section 2.6.1. Let $G_N$ represent the matrix of coefficients $G_{Nkl}(t)$, and $\xi$ the vector of basis functions $\xi_k(r,t)$. Since the matrix $G_N$ is Hermitian, ie. $G_{Nkl} = G^*_{Nlk}$, we can write $G_N$ in the diagonal form

$$G_N = X^* D X \tag{2.95}$$

where $D$ is a diagonal matrix, and $X$ is a unitary matrix. Then defining $\zeta \equiv X^* \xi$ we can write the thermal density $\tilde{n}$ in the form

$$\tilde{n}(r,t) = \sum_q D_q(t) \zeta_q^*(r,t) \zeta_q(r,t). \tag{2.96}$$
It is interesting to compare this with the thermal density $\tilde{n}$ in the HFB formalism given by (2.52). Since $X$ is unitary,

$$\int d\mathbf{r} \zeta^*(\mathbf{r}, t) \zeta(\mathbf{r}, t) = \int d\mathbf{r} X^T \zeta^*(\mathbf{r}, t) \zeta(\mathbf{r}, t) X = X^T X = I,$$

(2.97)
i.e. $\int d\mathbf{r} \zeta^*_q(\mathbf{r}, t) \zeta_q(\mathbf{r}, t) = 1$, in contrast to the normalisation condition (2.54) for the quasi-particle amplitudes $u_q$ and $v_q$ in HFB. One might be tempted to associate $u_q \equiv \varsigma_q$ and $v_q \equiv 0$, but this implies $\tilde{m} \equiv 0$ and is inconsistent with (2.94) where $\tilde{m}$ is certainly not zero. We conclude therefore that, whilst similar, this theory is not equivalent to the HFB formalism discussed in section 2.6.1. In HFB we assume the existence of a non-interacting quasi-particle basis, whereas no such assumption has been made here.

### 2.7 Number-conserving Theories

As already mentioned, the symmetry-breaking approach breaks the $U(1)$ symmetry, and hence overall number conservation is violated. One overcomes this problem by working in the Grand-Canonical ensemble where the self-consistent calculation of the chemical potential $\mu$ and suitable normalisation of the quasi-particle amplitudes and of the condensate fixes the overall problem. However this has implications for the fluctuations with variance $\delta^2_{n_0} = \left( 1 - \left( \frac{T}{T_c} \right)^\eta \right)^2 \bar{N}^2$, where $\eta$ is a trap-dependent exponent, and implies the unusual scaling of $\delta^2_{n_0} \propto \bar{N}^2$ [12, 13] leading to the Grand-Canonical catastrophe. This arises from the inconsistency of the symmetry-breaking treatment for a finite number of particles.

In number-conserving approaches, one maintains the $U(1)$ symmetry (and hence maintains particle conservation) by avoiding the broken symmetry ansatz. One also aims to achieve a systematic expansion of the Hamiltonian which facilitates a perturbative approach. To lowest order, the symmetry-breaking and number-conserving approaches lead to essentially the same equations, namely the GPE (2.42) and the BdGEs (2.50) in the Bogoliubov approximation. There are various ways by which this might be achieved:

#### 2.7.1 The approach due to C. W. Gardiner

**Homogeneous Bose gas** In his paper [22], C. W. Gardiner considers the Hamiltonian (in momentum space)

$$\hat{H} = \sum_\mathbf{k} \hbar \omega_\mathbf{k} \hat{b}_\mathbf{k}^\dagger \hat{b}_\mathbf{k} + \frac{g}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \hat{b}_{\mathbf{k}_1}^\dagger \hat{b}_{\mathbf{k}_2} \hat{b}_{\mathbf{k}_3} \hat{b}_{\mathbf{k}_4} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4}.$$

(2.98)
He defines an annihilation operator $\hat{A}$ for the total number of particles, thus $\hat{N} = \hat{A}^\dagger \hat{A}$ is the overall number operator. He defines phonon creation and annihilation operators $\hat{\beta}^\dagger_k$ and $\hat{\beta}_k$ for the excitations in mode $k$ in terms of the single-particle operators $\hat{a}_k$ by

$$\hat{\beta}_k \equiv \frac{1}{\sqrt{N}} \hat{b}_0 \hat{b}_k$$

and shows that

$$\hat{b}_0 = \hat{A} \left( 1 - \frac{\sum_{k \neq 0} \hat{\nu}_k}{2N} \right) \approx \hat{A}$$

in the limit $N \to \infty$. The operators $\hat{\beta}_k$ obey the Bose commutator relations (approximately) to order $1/N$, i.e.

$$[\hat{\beta}_k, \hat{\beta}_k^\dagger] = \delta_{k,k'} - \frac{1}{N} \hat{b}_k \hat{b}_{k'} \approx \delta_{k,k'}$$

Inhomogeneous Bose gas  In the spatially inhomogeneous case, the Hamiltonian may be written as

$$\hat{H} = \int dr \left( \hat{\psi}^\dagger(r,t) \hat{h}(r) \hat{\psi}(r,t) + \frac{g}{2} \int dr \hat{\psi}^\dagger(r,t) \hat{\psi}^\dagger(r,t) \hat{\psi}(r,t) \hat{\psi}(r,t) \right)$$

He reformulates the system Hamiltonian (2.101), and the Bose field operator $\hat{\psi}(r,t)$, which is expanded in terms the annihilation operator $\hat{A}$, a condensate wave-function $\phi$, and a phonon field operator $\hat{\Lambda}$ (see below), performing an asymptotic expansion of the Hamiltonian in powers of $\sqrt{N}$,

$$\hat{H} \approx \hat{N} H_0 + \sqrt{N} \hat{H}_1 + \hat{H}_2$$

where

$$H_0 = \int dr \left( \phi^* \hat{h} \phi + \frac{1}{2} g N |\phi|^4 \right)$$
$$\hat{H}_1 = \int dr \left( \hat{\Lambda}^\dagger \hat{h} \phi + \hat{h} \phi^* + g N |\phi|^2 \left( \phi \hat{\Lambda}^\dagger + \phi^* \hat{\Lambda} \right) \right)$$
$$\hat{H}_2 = \int dr \left( \hat{\Lambda}^\dagger \hat{h} \hat{\Lambda} + \frac{1}{2} g N \left( \phi^2 \hat{\Lambda}^\dagger \hat{\Lambda}^\dagger + \phi^* \hat{\Lambda} \hat{\Lambda} \right) + \hat{\Lambda}^\dagger \hat{\Lambda} \left( 2gN |\phi|^2 - \mu \right) - \frac{1}{2} g N |\phi|^4 \right)$$

and where

$$\mu = \int dr \left( \phi^*(r,t) \hat{h}(r) \phi(r,t) + g N |\phi(r,t)|^4 \right)$$

The field particle operator is approximated by

$$\hat{\psi}(r,t) \approx \hat{A} \left( \phi(r,t) + \frac{1}{\sqrt{N}} \hat{\Lambda}(r,t) \right)$$
where $\phi(r)$ is the condensate wave-function normalised to unity, and $\hat{\Lambda}(r)$ is a phonon field operator defined by

$$\hat{\Lambda}(r,t) \equiv \sum_k \phi_k(r) \hat{b}_k.$$  \hfill (2.106)

Choosing $\phi$ to minimize $\hat{H}$ subject to the normalization condition $\int d\mathbf{r} |\phi(r,t)|^2 = 1$, he obtains the time-independent Gross-Pitaevskii equation

$$\left(\hat{h} + gN |\phi(r)|^2\right) \phi(r) = \mu \phi(r)$$ \hfill (2.107)

Making the Bogoliubov transformation

$$b_k = \sum_m (c_{km} \hat{a}_m + d_{km} \hat{a}_m^\dagger)$$ \hfill (2.108)

we can write

$$\hat{\Lambda}(r,t) = \sum_m \left( u_m(r,t) \hat{a}_m + v_m^*(r,t) \hat{a}_m^\dagger \right)$$ \hfill (2.109)

where

$$u_m(r,t) \equiv \sum_k c_{km} \phi(r) \quad \text{and} \quad u_m(r,t) \equiv \sum_k c_{km} \phi(r)$$ \hfill (2.110)

in terms of quasi-particles with creation and annihilation operators $\hat{a}_k^\dagger$ and $\hat{a}_k$, we can then write the Hamiltonian $\hat{H}_2$ in diagonal form

$$\hat{H}_2 = \hbar \omega_g(N) + \sum_m \hbar \epsilon_m(N) \hat{a}_k^\dagger \hat{a}_k$$ \hfill (2.111)

where $\epsilon_m(N)$ are the excitation energies of the quasi-particles.

**Applicability**  In view of the approximations implied by the number-conserving ansatz (2.105), and the omission of the thermal density (this is essentially the GPE), this theory is only valid at $T = 0$.

### 2.7.2 The approach due to S. A. Morgan

A number-conserving, finite-temperature analysis incorporating second-order perturbation theory was performed by S. A. Morgan [23, 24]. In his analysis, he defines the number conserving operators by $\hat{\alpha}_k = \hat{a}_0^\dagger \hat{b}_k$ where $\hat{a}_0 = \left(\hat{N}_0 + 1\right)^{1/2} \hat{b}_0$ with $\hat{N}_0 = \hat{b}_0^\dagger \hat{b}_0$ the operator for the condensate number, and $\hat{b}_k$ are the mode operators for the basis functions $\{ \phi_i(r) \}$ in the Bose Hamiltonian

$$\hat{H}(t) = \sum_{k,l=1}^{\infty} \langle k | \hat{A} | l \rangle \hat{b}_k^\dagger \hat{b}_l + \frac{1}{2} \sum_{k,l,m,n=1}^{\infty} \langle kl | U^{(S)} | mn \rangle \hat{b}_k^\dagger \hat{b}_l^\dagger \hat{b}_n \hat{b}_m$$ \hfill (2.112)
where \( \langle k|\hat{h}|l \rangle = \int d\mathbf{r} \phi^*_k(\mathbf{r}) \hat{h}(\mathbf{r}) \phi_l(\mathbf{r}) \), and \( U^{(S)} \) is the symmetrised interaction potential defined by \( \langle kl|U^{(S)}|mn \rangle = \frac{1}{2}[\langle kl|U|mn \rangle + \langle lk|U|mn \rangle] \) with

\[
\langle kl|U|mn \rangle = \int d\mathbf{r} \int d\mathbf{r}' \phi^*_k(\mathbf{r}) \phi_l^*(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \phi_m(\mathbf{r}') \phi_n(\mathbf{r})
\]

where \( U(\mathbf{r} - \mathbf{r}') \) is the effective atomic potential. He rewrites the Hamiltonian as follows

\[
\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4
\]

where

\[
\hat{H}_0 = \sqrt{N_0} \left( \langle 0|\hat{h}|0 \rangle + \frac{1}{2} N_0 \langle 00|U^{(S)}|00 \rangle \right)
\]

\[
\hat{H}_1 = \sqrt{N_0} \sum_{k \neq 0} \left( \langle k|\hat{h}|0 \rangle + \frac{1}{2} \langle k0|U^{(S)}|00 \rangle \right) \hat{b}^\dagger_k + \text{h.c.}
\]

\[
\hat{H}_2 = \sum_{k,l \neq 0} \left( \langle k|\hat{h}|l \rangle - \lambda \delta_{k,l} + 2 N_0 \langle 0k|U^{(S)}|l0 \rangle \right) \hat{b}^\dagger_k \hat{b}^\dagger_l + \sum_{k,l \neq 0} \left( \frac{N_0}{2} \langle kl|U^{(S)}|00 \rangle \hat{b}^\dagger_k \hat{b}^\dagger_l + \text{h.c.} \right) + \lambda \langle \hat{N}_{ex} \rangle
\]

\[
\hat{H}_3 = \sum_{k,l,m \neq 0} \left( \sqrt{N_0} \langle kl|U^{(S)}|m0 \rangle \hat{b}^\dagger_k \hat{b}^\dagger_l \hat{b}_m + \text{h.c.} \right)
\]

\[
\hat{H}_4 = \sum_{k,l,m \neq 0} \frac{1}{2} \langle kl|U^{(S)}|mn \rangle \hat{b}^\dagger_k \hat{b}^\dagger_l \hat{b}_m \hat{b}_n
\]

is the number operator for the non-condensate. \( \langle \hat{N}_{ex} \rangle \) is the ensemble-averaged quantum expectation value, and is the mean occupation for the non-condensate. \( N_0 \) is the mean condensate population, and is defined by \( N_0 = N - \langle \hat{N}_{ex} \rangle \).

He first considers the terms in \( \hat{H} \) to quadratic order, ie. \( \hat{H}_0, \hat{H}_1, \) and \( \hat{H}_2 \). The parameter \( \lambda \) is defined by \( \lambda \equiv \langle 0|\hat{h}|0 \rangle + N_0 \langle 00|U^{(S)}|00 \rangle \) and is merely the condensate eigenstate as calculated for the GPE. Minimization of \( H_0 \) yields the GPE

\[
\langle k|\hat{h}|0 \rangle + N_0 \langle k0|U^{(S)}|00 \rangle = \lambda \delta_{k0}
\]

which in the position representation using the contact potential approximation \( U(\mathbf{r}) = g \delta(\mathbf{r}) \) with \( g = 4\pi \hbar^2 a_s / m \), \( \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \) where \( a_s \) is the s-wave scattering length, and \( m \) is the atomic mass is given by

\[
\left( \hat{h} + g N |\phi_0(\mathbf{r})|^2 \right) \phi_0(\mathbf{r}) = \lambda \phi_0(\mathbf{r}).
\]
The quantity $\lambda$ is introduced as the Lagrange multiplier for the constraint on the normalization $\int d\mathbf{r} \left| \zeta_0(\mathbf{r}) \right|^2 = 1$ (when we perform the functional differentiation).

The basis functions $\{ \phi_k(\mathbf{r}), k \neq 0 \}$ describe the non-condensate and must be chosen to be orthogonal to the condensate wave-function $\phi_0(\mathbf{r})$. A convenient choice for these functions in a trapped gas is the GPE basis defined by the solution of the GPE

$$\left( \hat{h} + gN \left| \phi_0(\mathbf{r}) \right|^2 \right) \phi_k(\mathbf{r}) = \lambda_k \phi_k(\mathbf{r})$$

where $\lambda_k$ is the energy of the basis state. The diagonalisation of $\hat{H}_2$ may be readily performed by writing

$$\hat{H}_2 = \sum_{k,l \neq 0} \left( \mathcal{L}_{kl} \hat{b}_k^\dagger \hat{b}_l + \frac{1}{2} \mathcal{M}_{kl} \hat{b}_k^\dagger \hat{b}_l^\dagger + \frac{1}{2} \mathcal{M}_{kl}^* \hat{b}_k \hat{b}_l \right) + \lambda \langle \hat{N}_{ex} \rangle$$

where

$$\mathcal{L}_{kl} = \langle k | \hat{h} | l \rangle - \lambda \delta_{kl} + 2N_0 \langle 0k | U^{(S)} | 0l \rangle$$

$$\mathcal{M}_{kl} = N_0 \langle kl | U^{(S)} | 00 \rangle$$

and by applying the Bogoliubov transformation

$$\hat{a}_k = \sum_{l \neq 0} \left( U_{kl} \hat{b}_l + V_{kl}^* \hat{b}_l^\dagger \right)$$

where the matrices $U$ and $V$ satisfy the orthogonality and symmetry conditions

$$UU^\dagger - VV^\dagger = 1, \quad UV^T - VU^T = 0$$

in order to preserve the Bose commutation relations. Defining the vectors $u_p \equiv [u_{p1} \ldots u_{pM}]^T$ and $v_p \equiv [v_{p1} \ldots v_{pM}]^T$, we obtain the BdGEs

$$\begin{bmatrix} \mathcal{L} & \mathcal{M} \\ -\mathcal{M}^* & -\mathcal{L}^* \end{bmatrix} \begin{bmatrix} u_p \\ v_p \end{bmatrix} = \epsilon_p \begin{bmatrix} u_p \\ v_p \end{bmatrix}$$

where $\mathcal{L}$ and $\mathcal{M}$ are the matrices with elements $\mathcal{L}_{kl}$ and $\mathcal{M}_{kl}$ respectively, which constitute the necessary and sufficient conditions for the quasi-particle transformations to diagonalise the BdGEs. The Hamiltonian $\hat{H}_2$ can then be written

$$\hat{H}_2 = \sum_{k \neq 0} \left( \epsilon_k \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} (\epsilon_i - \mathcal{L}_{ii}) \right) + \lambda \langle \hat{N}_{ex} \rangle$$

where the quasi-particle energies are given by

$$\epsilon_p = \begin{bmatrix} u_p & -v_p^* \end{bmatrix} \begin{bmatrix} \mathcal{L} & \mathcal{M} \\ -\mathcal{M}^* & -\mathcal{L}^* \end{bmatrix} \begin{bmatrix} u_p \\ v_p \end{bmatrix}.$$
He demonstrates that the excitation spectrum is gapless by showing that the energy of a quasi-particle in the homogeneous limit tends to zero as its momentum tends to zero.

In the position representation, we write the quasi-particle amplitudes as

\[ u_p(r) = \sum_{k \neq 0} U_{pk} \phi_k(r) \quad , \quad v_p^*(r) = \sum_{k \neq 0} V_{pk}^* \phi_k(r) \]  \hspace{1cm} (2.128)

for an arbitrary complete basis \( \{ \phi_k(r) \} \), with orthonormality and symmetry relations

\[
\int dr \left( u_p(r) u_q^*(r) - v_p(r) v_q^*(r) \right) = \delta_{pq}
\]

\[
\int dr \left( u_p(r) v_q(r) - u_q(r) v_p(r) \right) = 0
\]  \hspace{1cm} (2.129)

yielding the BdGEs (using the contact potential)

\[
\begin{bmatrix}
\hat{\tilde{L}}(r) & M(r) \\
-M^*(r) & -\hat{\tilde{L}}^*(r)
\end{bmatrix}
\begin{bmatrix}
u_p(r) \\
v_p^*(r)
\end{bmatrix}
= \epsilon_p
\begin{bmatrix}
u_p(r) \\
v_p^*(r)
\end{bmatrix}
+ c_p
\begin{bmatrix}
\phi_0(r) \\
-\phi_0^*(r)
\end{bmatrix}.
\]  \hspace{1cm} (2.130)

Here

\[
\hat{\tilde{L}}(r) \equiv \hat{\tilde{h}}(r) - \lambda + 2N_0 g |\phi_0(r)|^2
\]

\[
M(r) \equiv N_0 g \phi_0^2(r)
\]  \hspace{1cm} (2.131)

and

\[
c_p \equiv \int dr N_0 g |\phi_0(r)|^2 \left( \phi_0^*(r) u_p(r) + \phi_0(r) v_p(r) \right) .
\]  \hspace{1cm} (2.132)

Given the usual forms for the BdGEs

\[
\begin{bmatrix}
\hat{\tilde{L}}(r) & M(r) \\
-M^*(r) & -\hat{\tilde{L}}^*(r)
\end{bmatrix}
\begin{bmatrix}
\tilde{u}_p(r) \\
\tilde{v}_p(r)
\end{bmatrix}
= \epsilon_p
\begin{bmatrix}
\tilde{u}_p(r) \\
\tilde{v}_p(r)
\end{bmatrix}
\]  \hspace{1cm} (2.133)

one can find the solutions to the BdGEs (2.130) by removing the projection onto the condensate, we have the following relationship

\[
\begin{bmatrix}
u_p(r) \\
v_p^*(r)
\end{bmatrix}
= \begin{bmatrix}
\tilde{u}_p(r) \\
\tilde{v}_p(r)
\end{bmatrix}
- \frac{c_p}{\epsilon_p}
\begin{bmatrix}
\phi_0(r) \\
-\phi_0^*(r)
\end{bmatrix}
\]  \hspace{1cm} (2.134)

thus allowing the BdGEs to be solved in a complete basis set \( \{ \phi_k(r) \} \) which is not necessarily orthogonal to the condensate. Clearly for the GPE basis \( c_p = 0 \), i.e. the solutions to the BdGEs are always orthogonal to the condensate, but removal of the projection onto the condensate as prescribed above allows us to use any arbitrary complete basis.

To progress beyond the quadratic Hamiltonian, one needs to take into account the ensemble average \( \langle \hat{H}_2 \rangle \) of \( \hat{H}_2 \) when deriving the generalised GPE (GGPE). One then obtains the expression for the GGPE

\[
\langle k| \hat{h} |0 \rangle + N_0 \langle k0| U^{(S)} |00 \rangle + \sum_{p,q \neq 0} \left( 2 \langle kp| U^{(S)} |q0 \rangle \tilde{\eta}_{qp} + \frac{1}{2} \langle k0| U^{(S)} |pq \rangle \tilde{\eta}_{qp} \right) = \lambda_c \delta_{k0}
\]

\(^5\)If the basis chosen is not orthogonal to the condensate, we need an extra basis function in order to have a complete basis set.
where $\tilde{n}_{kl} \equiv \langle \hat{b}_k^\dagger \hat{b}_l \rangle$ is the one-body density matrix (normal average), and $\tilde{m}_{kl} \equiv \langle \hat{b}_k \hat{b}_l \rangle$ is the anomalous average. In the position representation, using the contact potential approximation, one obtains

$$
\left( \hat{h} + gN \left( |\phi_0(r)|^2 + 2\tilde{n}(r) \right) \right) \phi_0(r) + gN\tilde{m}(r)\phi_0^*(r) = \lambda_G\phi_0(r) \tag{2.135}
$$

which is just the GGPE (2.65) found using HFB, with the thermal and anomalous densities $\tilde{n}(r)$ and $\tilde{m}(r)$ given respectively by equations (2.59) and (2.60). This implies a change in $\hat{H}_1$ of

$$
\Delta \hat{H}_1 = -\sqrt{N_0} \sum_{k,l,m \neq 0} \left( 2 \langle mk | U^{(S)} | l0 \rangle \tilde{n}_{lk} + \langle m0 | U^{(S)} | kl \rangle \tilde{m}_{lk} \right) \hat{b}_k^\dagger + h.c. \tag{2.136}
$$

and in $\hat{H}_2$ of $\Delta \hat{H}_2 = \hat{H}_2(\tilde{\phi}_0(r)) - \hat{H}_2(\phi_0(r))$ where $\tilde{\phi}_0(r)$ denotes the solution of the GGPE, and $\phi_0(r)$ the solution of the ordinary GPE, thus

$$
\Delta \hat{H}_2 = \sum_{k,l \neq 0} \left[ \left( 2N_0 \langle 0k | U^{(S)} | 00 \rangle - 2N_0 \langle 0k | U^{(S)} | 0l \rangle + 2N_0 \langle 0l | U^{(S)} | 00 \rangle \right) \hat{b}_k^\dagger \hat{b}_l^\dagger + \text{h.c.} \right]
$$

$$
\approx \sum_{k,l \neq 0} \left( \langle 0k | U^{(S)} | 00 \rangle - \langle kl | U^{(S)} | 00 \rangle \right) \hat{b}_k^\dagger \hat{b}_l^\dagger + \text{h.c.}
$$

where

$$
\mathcal{L}_{\delta k,l} \equiv \langle k | \hat{h} | l \rangle - \langle k | \hat{h} | l \rangle - \lambda \delta_{kl} + 2N_0 \langle 0\bar{k} | U^{(S)} | 0 \rangle - 2N_0 \langle 0k | U^{(S)} | 0 \rangle
$$

$$
\mathcal{M}_{\delta k,l} \equiv N_0 \langle 0\bar{l} | U^{(S)} | 00 \rangle - N_0 \langle kl | U^{(S)} | 00 \rangle.
$$

He treats the non-quadratic terms, given by

$$
\hat{H}_{\text{pert}} = \hat{H}_3 + \hat{H}_4 + \Delta \hat{H}_1 + \Delta \hat{H}_2 \tag{2.139}
$$

using first- and second- order perturbation theory in a quasi-particle basis [23, 24] (see also [57]).

**First Order Perturbation Theory in S. A. Morgan’s Treatment** [23, 24] The energy shift to a quasi-particle number state $|S\rangle = |n_1 \ldots n_k \ldots \rangle$ is given by $E_{\text{pert}}(S, 1) = \langle S | \Delta \hat{H}_{\text{pert}} | S \rangle$. Clearly $\langle S | \Delta \hat{H}_3 | S \rangle = \langle S | \Delta \hat{H}_1 | S \rangle = 0$, and

$$
E_4 = \langle \hat{H}_4 \rangle = \frac{1}{2} \sum_{i,j,k,l \neq 0} \langle ij | U^{(S)} | kl \rangle \left( \tilde{n}_{ki} \tilde{n}_{lj} + \tilde{n}_{li} \tilde{n}_{kj} + \tilde{m}_{ij}^* \tilde{m}_{kl} \right)
$$
Chapter 2. Background Theory

since \( \langle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \rangle = \tilde{n}_{ki} \tilde{n}_{lj} + \tilde{n}_{il} \tilde{n}_{kj} + \tilde{m}_{ij}^* \tilde{n}_{kl} \). The energy shift for quasi-particle \( p \) is then given by

\[
\Delta E_4(p) = E_4(n_1 \ldots n_p + 1 \ldots) - E_4(n_1 \ldots n_p \ldots)
\]

which, in the position representation, can be written as

\[
\Delta E_4 = g \int dr \left( 2\tilde{n}(r)\Delta \tilde{n}_p(r) + 2\tilde{m}(r)\Delta \tilde{m}_p(r) \right)
\]

where

\[
\begin{align*}
\tilde{n}(r) & \equiv \sum_{p \neq 0} (n_p |u_p(r)|^2 + (n_p + 1) |v_p(r)|^2) \\
\Delta \tilde{n}_p(r) & \equiv |u_p(r)|^2 + |v_p(r)|^2 \\
\tilde{m}(r) & \equiv \sum_{p \neq 0} (2n_p + 1)u_p(r)v_p^*(r) \\
\Delta \tilde{m}_p(r) & \equiv 2u_p(r)v_p^*(r)
\end{align*}
\]

Here \( \Delta \tilde{n}_p(r) \) is the change in \( \tilde{n}(r) \) with \( n_p \rightarrow n_p + 1 \), and \( \Delta \tilde{m}_p(r) \) the change in \( \tilde{m}(r) \) with \( n_p \rightarrow n_p + 1 \). The change in the contribution to the energy of the system by \( \Delta \hat{H}_2 \) (given by equation (2.137)) when we add a quasi-particle to mode \( p \), \( \Delta E_{\text{shape}}(p) \) can be written in the position representation as

\[
\Delta E_{\text{shape}}(p) = N_0 g \int dr \left( \phi_0^2(r) - \phi_0^2(r) \right) \left( 2\Delta \tilde{n}_p(r) + \Delta \tilde{m}_p(r) \right) - \left[ c_p \int dr \left( \phi_0^2(r) - \phi_0^2(r) \right) (u_p^*(r) + v_p^*(r)) + \text{c.c.} \right].
\]

Both \( \Delta E_4(p) \) and \( \Delta E_{\text{shape}}(p) \) have been calculated as the change in energy of the system when a quasi-particle is created in mode \( p \). This change in the quasi-particle distribution must, however, be accompanied by a change in the condensate population, since the total number of particles is fixed, therefore the creation of a quasi-particle via \( n_p \rightarrow n_p + 1 \) also leads to a change in the energy of the quadratic Hamiltonian given by

\[
\Delta (H_0 + E_2) = -\sum_{i,j \neq 0} \delta_{ij} \Delta \tilde{n}_{ij}(p).
\]

This leads to a perturbative shift in the quasi-particle energy given in the position representation by

\[
\Delta E_{\lambda}(p) = -(\lambda_G - \lambda) \int dr \Delta \tilde{n}_p(r).
\]

The energy shifts given by \( \Delta E_4(p) \), \( \Delta E_{\text{shape}}(p) \) and \( \Delta E_{\lambda}(p) \) are quadratic in \( U_{pi} \) and \( V_{pi} \) for mode \( p \), and may therefore be incorporated into the BdGEs (2.125), where the new matrices \( \mathcal{L} \) and \( \mathcal{M} \) are defined by

\[
\begin{align*}
\mathcal{L}_{ij} & \equiv \langle i | \hat{h} | j \rangle - \lambda_G \delta_{k,l} + 2N_0 \langle 0i | U^{(S)} | j0 \rangle + \sum_{k,l \neq 0} 2 \langle ki | U^{(S)} | jl \rangle \tilde{n}_{lk} \\
\mathcal{M}_{ij} & \equiv N_0 \langle ij | U^{(S)} | 00 \rangle + \sum_{k,l \neq 0} \langle ij | U^{(S)} | kl \rangle \tilde{m}_{kl}.
\end{align*}
\]

The contribution from \( \Delta E_{\text{shape}}(p) \) is implied, since the index 0 here refers to a solution of the GPE, and the basis states are orthogonal to this.
Ordinary perturbation amounts to the simple evaluation of the expressions for $\Delta E_4(p)$, $\Delta E_{\text{shape}}(p)$ and $\Delta E_\lambda(p)$ using quasi-particle energies, and transformation coefficients calculated from the quadratic BdGEs (i.e. ordinary BdGEs where $L_{ij} = \langle i | \hat{h} | j \rangle - \lambda \delta_{k,l} + 2N_0 \langle 0i | U^{(S)} | j0 \rangle$ and $M_{ij} = N_0 \langle ij | U^{(S)} | 00 \rangle$). Self-consistent perturbation theory, on the other hand, entails the exact diagonalisation of the generalised BdGEs with $L_{ij}$ and $M_{ij}$ as above. Comparison of the normal $L_{ij}$ and $M_{ij}$ with the generalised $L_{ij}$ and $M_{ij}$ shows that there are three types of correction introduced by $\Delta E_4(p)$, $\Delta E_{\text{shape}}(p)$ and $\Delta E_\lambda(p)$:

1. Condensate energy $\lambda$ and shape $\phi_0(r)$ are upgraded to values appropriate to GGPE

2. Direct and exchange collisions are included between non-condensate atoms and via the term $\sum_{k,l \neq 0} 2 \langle ki | U^{(S)} | jl \rangle \bar{n}_{lk}$ in $L_{ij}$

3. The anomalous average $\bar{m}_{ij}$ is introduced into the off-diagonal terms $M_{ij}$. We can interpret this correction as follows:- it upgrades the condensate-condensate interactions which appear in leading order contribution to $M_{ij}$ so that these are described by the many-body T-matrix.

We note that the change to coefficients $L_{ij}$ and $M_{ij}$ which are introduced by $\Delta E_4(p)$ are exactly the same as would have been obtained using the factorisation approximation used in HFB on the operators appearing in $\hat{H}_4$. Hence this approximation on the product of four operators is equivalent to self-consistent first-order perturbation theory, and is therefore justified to this order of calculation. Wick’s Theorem is concerned with operator averages, and hence the equations from first-order perturbation theory and HFB are identical - this follows since by Wick’s theorem, all ensemble averages of terms having an odd number of fluctuation creation and annihilation operators $\hat{\eta}^\dagger$ and $\hat{\eta}$ are zero, whereas those with an even number may be evaluated yielding the same terms.

**Second Order Perturbation Theory in S. A. Morgan’s Treatment [23, 24]** The energy shift of a quasi-particle state $|S\rangle$ from second order perturbation theory is

$$E_{\text{pert}}(S, 2) = \sum_{R \neq S} \frac{|\langle R | \hat{H}_{\text{pert}} | S \rangle|^2}{E_S - E_R}$$

(2.145)

where $E_S$ and $E_R$ are energies of the system calculated from the quadratic Hamiltonian.
One can neglect the contribution from $\hat{H}_4 + \Delta \hat{H}_2$ at this order of perturbation theory, thus we need only consider the modified cubic Hamiltonian $\hat{H}_3' = \hat{H}_3 + \Delta \hat{H}_1$. We can write

$$\hat{H}_3' = \hat{H}_3 + \Delta \hat{H}_1 = \sum_{i,j,k \neq 0} (A_{ijk} \hat{a}_i \hat{a}_j \hat{a}_k + B_{ijk} \hat{a}_i^\dagger \hat{a}_j \hat{a}_k) + \sum_{i \neq 0} C_i \hat{a}_i + \text{h.c.} \quad (2.146)$$

where

$$A_{ijk} = \sqrt{N_0} \sum_{m,n,q \neq 0} \langle q0 | U^{(S)} | mn \rangle V_{iq} U_{jn} U_{km} + \langle mn | U^{(S)} | q0 \rangle U_{iq} V_{jn} V_{km} \quad (2.147)$$

$$B_{ijk} = \sqrt{N_0} \sum_{m,n,q \neq 0} \left[ \langle q0 | U^{(S)} | mn \rangle \left( U_{iq}^* U_{jn} U_{km} + V_{in}^* V_{jq} U_{km} + V_{in}^* U_{jn} V_{km} \right) \right.
+ \left. \langle mn | U^{(S)} | q0 \rangle \left( U_{in}^* U_{jq} V_{km} + U_{in}^* V_{jn} U_{qk} + V_{iq} V_{jn} V_{km} \right) \right] \quad (2.148)$$

and

$$C_i = - \sum_{q \neq 0} \left( B_{qqi} + B_{qiq} \right) n_q \quad (2.149)$$

The modified cubic Hamiltonian gives a contribution to the energy of

$$E_3 = \frac{1}{6} \sum_{i,j,k \neq 0} \left| A_{ijk}^{P3} \right|^2 (n_i n_j n_k - (n_i + 1)(n_j + 1)(n_k + 1)) / (\epsilon_i + \epsilon_j + \epsilon_k) + \frac{1}{2} \sum_{i,j,k \neq 0} |B_{ijk} + B_{ikj}|^2 ((n_i + 1)n_j n_k - n_i (n_j + 1)(n_k + 1)) / (\epsilon_j + \epsilon_k - \epsilon_i)
- \sum_{i \neq 0} C_i + \sum_j \left( B_{jji} + B_{jjj} \right) n_j / \epsilon_i \quad (2.150)$$

where $A_{ijk}^{P3} \equiv A_{ijk} + A_{ikj} + A_{jik} + A_{kij} + A_{kji}$ (omitting terms which are negligible in the thermodynamic limit). The contribution to the energy of a quasi-particle is given by the change in $E_3$ as $n_p \to n_p + 1$, $\Delta E_3(p) = E_3(n_1 \ldots n_p + 1 \ldots) - E_3(n_1 \ldots n_p \ldots)$, hence [23, 24]

$$\Delta E_3(p) = \sum_{i,j \neq 0} \left[ - \frac{|A_{pji}^{P3}|^2 (1 + n_i + n_j)}{2(\epsilon_p + \epsilon_i + \epsilon_j)} + \frac{|B_{pj} + B_{pji}|^2 (1 + n_i + n_j)}{2(\epsilon_p - \epsilon_i - \epsilon_j)} + \frac{|B_{ijp} + B_{ipj}|^2 (n_j - n_i)}{(\epsilon_p - \epsilon_i + \epsilon_j)} \right]. \quad (2.151)$$

Although this expression has been derived for pure states, it may be re-interpreted as a thermal average. Thermal averages are calculated via the grand canonical partition function $Z_c = \sum_{\{n_i\}} \exp(-\beta E_i \{n_i\})$, where $E_i \{n_i\} = H_0 \{n_i\} + E_2 \{n_i\}$. To a good approximation, however, they can be obtained simply by replacing the condensate and quasi-particle populations with their thermal averages given by the Bose-Einstein distribution $n_p(T) = 1/(Z^{-1} \exp(\beta \epsilon_p) - 1)$ with fugacity $Z \equiv \exp(\beta(\mu - \lambda))$, where $\mu$ is the chemical potential.

The physical interpretation of $\Delta E_3(p)$ is that it introduces a T-matrix into the description of the condensate-non-condensate collisions. The first term in the above equation
corresponds to the simultaneous annihilation or creation of three quasi-particles. The second term represents Beliaev processes in which a single quasi-particle spontaneously decomposes into two others. The final term corresponds to Landau processes in which two quasi-particles collide and coalesce to form a single quasi-particle (essentially the reverse of a Beliaev process). Beliaev processes can occur at zero temperature, and are found to be dominant in the low temperature regime, whereas Landau processes cannot occur at zero temperature (because there are no excited quasi-particles at zero temperature), but dominate at high temperatures. The existence of these processes implies that the quasi-particles have a finite life-time. \( \Delta E_3(p) \) can be used for a trapped gas to calculate the time evolution of a quasi-particle, and to determine its lifetime. We note that \( \Delta E_3(p) \) is a quadratic form in the quasi-particle transformation coefficients \( U_p \) and \( V_p \) for mode \( p \).

We can write \( \Delta E_3(p) \) in the form

\[
\Delta E_3(p) = \begin{bmatrix} u_p & -v_p^* \end{bmatrix} \begin{bmatrix} \Delta \mathcal{L}(\epsilon_p) & \Delta \mathcal{M}(\epsilon_p) \\ -\Delta \mathcal{M}^*(-\epsilon_p) & -\Delta \mathcal{L}^*(-\epsilon_p) \end{bmatrix} \begin{bmatrix} u_p \\ v_p \end{bmatrix}
\]

where

\[
\Delta \mathcal{L}_{ij}(\epsilon_p) = \sum_{k,m \neq 0} \left[ \frac{1+n_k+n_m}{2} \left( \frac{\tilde{A}_{ikm}^* \tilde{A}_{jkm}}{\epsilon_p-(\epsilon_k+\epsilon_m)} - \frac{\tilde{B}_{ikm}^* \tilde{B}_{jkm}}{\epsilon_p+\epsilon_k+\epsilon_m} \right) + (n_m-n_k)\frac{\tilde{C}_{ikm}^* \tilde{C}_{jkm}}{\epsilon_p+\epsilon_m-\epsilon_k} \right]
\]

\[
\Delta \mathcal{M}_{ij}(\epsilon_p) = \sum_{k,m \neq 0} \left[ \frac{1+n_k+n_m}{2} \left( \frac{\tilde{A}_{ikm} \tilde{B}_{jkm}^*}{\epsilon_p-(\epsilon_k+\epsilon_m)} - \frac{\tilde{B}_{ikm}^* \tilde{A}_{jkm}}{\epsilon_p+\epsilon_k+\epsilon_m} \right) + (n_m-n_k)\frac{\tilde{C}_{ikm} \tilde{C}_{jkm}^*}{\epsilon_p+\epsilon_m-\epsilon_k} \right]
\]

where, in the position representation using the contact potential approximation

\[
\begin{align*}
\tilde{A}_{ikm} &= 2\sqrt{N_0} \int d\mathbf{r} \phi_i^*(\mathbf{r}) \left[ \phi_0^*(\mathbf{r}) u_k(\mathbf{r}) u_m(\mathbf{r}) + \phi_0^*(\mathbf{r}) (u_k(\mathbf{r}) v_m(\mathbf{r}) + v_k(\mathbf{r}) u_m(\mathbf{r})) \right] \\
\tilde{B}_{ikm} &= 2\sqrt{N_0} \int d\mathbf{r} \phi_i(\mathbf{r}) \left[ \phi_0(\mathbf{r}) v_k(\mathbf{r}) v_m(\mathbf{r}) + \phi_0(\mathbf{r}) (u_k(\mathbf{r}) v_m(\mathbf{r}) + v_k(\mathbf{r}) u_m(\mathbf{r})) \right] \\
\tilde{C}_{ikm} &= 2\sqrt{N_0} \int d\mathbf{r} \phi_i(\mathbf{r}) \left[ \phi_0(\mathbf{r}) u_k^*(\mathbf{r}) v_m(\mathbf{r}) + \phi_0(\mathbf{r}) (u_k^*(\mathbf{r}) u_m(\mathbf{r}) + v_k^*(\mathbf{r}) v_m(\mathbf{r})) \right].
\end{align*}
\]

We note that \( \Delta \mathcal{L}_{ij}^*(\epsilon_p) = \Delta \mathcal{L}_{ij}(\epsilon_p) \), and \( \Delta \mathcal{M}_{ij}(\epsilon_p) = \Delta \mathcal{M}_{ij}(-\epsilon_p) \).

Since \( \Delta E_3(p) \) simply modifies the matrices \( \mathcal{L} \) and \( \mathcal{M} \) in the BdGEs (2.125), its calculation can be made self-consistent by including \( \Delta \mathcal{L}(\epsilon_p) \) and \( \Delta \mathcal{M}(\epsilon_p) \) in the BdGEs, and calculating them exactly. Including also the effects of \( \Delta E_4(p) \), \( \Delta E_{\text{shape}}(p) \) and \( \Delta E_\lambda(p) \), he obtains the generalised BdGEs

\[
\begin{bmatrix} \mathcal{L}(\epsilon_p) & \mathcal{M}(\epsilon_p) \\ -\mathcal{M}^*(-\epsilon_p) & -\mathcal{L}^*(-\epsilon_p) \end{bmatrix} \begin{bmatrix} u_p \\ v_p \end{bmatrix} = \epsilon_p \begin{bmatrix} u_p \\ v_p \end{bmatrix}
\]
where $\mathcal{L}(\epsilon_p)$ and $\mathcal{M}(\epsilon_p)$ are the matrices with elements

\[
\mathcal{L}_{ij}(\epsilon_p) = \mathcal{L}_{ij} + \Delta \mathcal{L}_{ij}(\epsilon_p) \quad \text{and} \quad \mathcal{M}_{ij}(\epsilon_p) = \mathcal{M}_{ij} + \Delta \mathcal{M}_{ij}(\epsilon_p)
\]  

(2.157)

with

\[
\mathcal{L}_{ij} \equiv \langle i | \hat{h} | j \rangle - \lambda \delta_{k,l} + 2 N_0 \langle 0 i | U^{(S)} | j 0 \rangle + \sum_{k,l \neq 0} 2 \langle ki | U^{(S)} | j l \rangle \tilde{n}_{lk} \\
\mathcal{M}_{ij} \equiv N_0 \langle ij | U^{(S)} | 00 \rangle + \sum_{k,l \neq 0} \langle ij | U^{(S)} | kl \rangle \tilde{n}_{kl}
\]  

(2.158)

We note the following:

1. The matrix to be diagonalised now depends on the quasi-particle energy, therefore a single matrix diagonalisation no longer yields the whole quasi-particle spectrum.

2. The factorisation approximation neglects all Beliaev and Landau processes which can occur in the non-condensate. These give a contribution to the energy of the order of $\Delta E_4(p)$ but neglect terms in $\Delta E_3(p)$ since by Wick’s theorem ensemble averages for terms involving an odd number of the fluctuation operators $\hat{\eta}$ and $\hat{\eta}^\dagger$ are identically zero. Therefore the factorisation approximation results in inconsistent treatment of the non-quadratic Hamiltonian, and hence $\Delta E_3(p)$ is required to remove IR divergences in the theory, leading to a gapless spectrum.

**Applicability**  The formalism of S. A. Morgan [23, 24] is directly applicable to the calculation of energy shifts using second-order perturbation theory to take into account the Beliaev and Landau processes. The disadvantage of this approach is that the generalised BdGEs (2.156) are difficult to solve and are quite computationally intensive. The other problem is that dynamic shifts in the quasi-particle energies are not taken into account, the reason being that the thermal density is static and therefore introduces an effective potential which modifies the energy shifts - for example, one would not expect Kohn’s theorem\(^6\) to be rigorously satisfied for the $m = 1$ mode. Rather one would expect the $m = 1$ mode frequency to be under-estimated by a few percent for $T \sim T_c/2$, depending on the interaction strength in the BEC.

This formalism is strictly time-independent in view of the way the energy shifts are introduced into the BdGEs (2.125) using the form (2.152) for the quasi-particle energy shifts. Therefore this formalism is not compatible with any time-dependent theory. In chapter 4

\(^6\)Kohn’s theorem states that for a harmonically trapped BEC, the dipole mode of the condensate (corresponding to the centre of mass oscillation), should occur at the harmonic oscillator frequency (see, for example, the review article [5]).
we shall explore an adaptation of this theory which uses the same expression (2.151) for the quasi-particle energy shifts, but which is also consistent with a time-dependent theory in which the condensate and thermal populations are always orthogonal.

The Approach due to Y. Castin and R. Dum

In their paper [25], Castin and Dum argue along the lines that in the case of the $U(1)$ symmetry-breaking approach, the state of the system is described by a coherent state, hence the atomic field operator has a non-zero expectation value ( [66], see also [22]). The mean value is thus a classical field characterising the condensate, and constitutes an explicit $U(1)$ symmetry-breaking as the condensate has a well-defined phase. But it should be noted that a coherent state is not a stationary state of the system since it does not have a well-defined number of particles. The Bogoliubov approach [67, 68] predicts a time divergence of quantum phase fluctuations. We can interpret this as a quantum phase spreading of the condensate which invalidates the linearization around the classical field very soon (as the number of particles is small). In their approach, Y. Castin and R. Dum [25] do not rely on symmetry-breaking, and thus avoid pathologies associated with phase fluctuations of the condensate. In their analysis, they use the contact potential approximation $U(r_1 - r_2) = g\delta(r_1 - r_2)$ where $g = 4\pi\hbar^2a_s/m$ and where $a_s$ is the s-wave scattering length, as already described.

The condensate wave-function [69] is described as the expectation value of the trace of the one-body density matrix $\rho_1(r, r, t) = \langle \hat{\psi}^\dagger(r, t)\hat{\psi}(r, t) \rangle$ where the one-body density matrix is given by

$$\rho_1(r, r', t) = \langle r | \hat{\rho}_1(t) | r' \rangle = \langle \hat{\psi}^\dagger(r, t)\hat{\psi}(r', t) \rangle \quad (2.159)$$

for the field operator $\hat{\psi}(r, t)$ in the Heisenberg picture. They assume that the number of particles $N$ is well-defined (so $Tr(\hat{\rho}_1) = N$) and suppose an $N$-particle system that is initially in thermal equilibrium at temperature $T$. A condensate is present if $\hat{\rho}_1$ has an eigenvector $|\phi\rangle$ with eigenvalue $N_c$ of the order of $N$, far exceeding all other eigenvalues, i.e. $\hat{\rho}_1 |\phi\rangle = N_c |\phi\rangle$. The condensate wave-function $|\phi\rangle$ is the exact state in which a macroscopic number $N_c$ of particles is condensed. Clearly $|\phi\rangle$ is normalised to unity, i.e. $\langle \phi | \phi \rangle = \int dr |\phi(r)|^2 = 1$. We are thus justified in splitting the field operator $\hat{\psi}(r, t)$ into a condensate part (macroscopic matrix elements), and a non-condensate part (accounts for non-condensed particles)

$$\hat{\psi}(r, t) = \phi(r, t)\hat{a}_c(t) + \eta(r, t) \quad (2.160)$$
where the condensate mode operator is given by

\[ \hat{a}_c(t) = \int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \]  \hspace{1cm} (2.161)

with \( \phi(\mathbf{r}, t) \) normalised to unity, i.e.

\[ \int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 = 1. \]  \hspace{1cm} (2.162)

In the Schrödinger picture \( \hat{a}_c(t) \) annihilates a particle in the condensate (wave-function \( \phi(\mathbf{r}, t) \)). Furthermore, \( \hat{a}_c(t) \) has matrix elements of the order of \( \sqrt{N_c} \) since the expectation value \( \langle \hat{a}_c^\dagger(t) \hat{a}_c(t) \rangle = N_c \).

The non-condensate part \( \hat{\eta}(\mathbf{r}, t) \) is obtained by the projection of the field operator \( \hat{\psi}(\mathbf{r}, t) \) orthogonally to \( \phi(\mathbf{r}, t) \):

\[ \hat{\eta}(\mathbf{r}, t) = \int d\mathbf{r}' \langle \mathbf{r} | \hat{Q}(t) | \mathbf{r}' \rangle \hat{\psi}(\mathbf{r}', t) = \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}', t) \hat{\psi}(\mathbf{r}', t) \]  \hspace{1cm} (2.163)

where the projection operator \( \hat{Q}(t) = 1 - |\phi\rangle \langle \phi| \) projects onto the one-particle states orthogonal to the condensate wave-function \( \phi \). In the position representation, the projection operator \( \hat{Q}(t) \) may be written as

\[ Q(\mathbf{r}, \mathbf{r}', t) = \delta(\mathbf{r} - \mathbf{r}') - \phi(\mathbf{r}, t)\phi^*(\mathbf{r}', t) \]  \hspace{1cm} (2.164)

Clearly \( \hat{\eta}(\mathbf{r}, t) \) is orthogonal to \( \phi(\mathbf{r}, t) \) since \( \int d\mathbf{r} \phi^* \hat{\eta} = \int d\mathbf{r} \phi^* \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}', t) \hat{\psi}(\mathbf{r}', t) = \int d\mathbf{r} \phi^* \hat{\psi} - (\int d\mathbf{r} \phi^* \phi) \int d\mathbf{r} \phi^* \hat{\psi} = 0 \) by the normalisation condition (2.162). Furthermore (2.163) shows that \( \hat{\eta}(\mathbf{r}, t) \) satisfies the quasi-bosonic commutation relations

\[ [\hat{\eta}(\mathbf{r}, t), \hat{\eta}^\dagger(\mathbf{r}', t)] = Q(\mathbf{r}, \mathbf{r}', t) \]  \hspace{1cm} (2.165)

From (2.160), (2.161), and (2.162), we see that \( \hat{\eta}(\mathbf{r}, t) \) commutes with \( \hat{a}_c^\dagger(t) \), i.e.

\[ [\hat{a}_c^\dagger(t), \hat{\eta}(\mathbf{r}, t)] = 0. \]  \hspace{1cm} (2.166)

They now write the Hamiltonian as a systematic expansion in powers of \( \sqrt{N}^{-1/2} \) and identify a small parameter by introducing the operator

\[ \hat{\Lambda}(\mathbf{r}, t) = \frac{1}{\sqrt{\hat{N}}} \hat{a}_c^\dagger(t) \hat{\eta}(\mathbf{r}, t) \]  \hspace{1cm} (2.167)

where \( \hat{N} \) is the total number operator. This has validity in the regime where the mean number of non-condensed atoms is very much less than the total number of atoms. In this
regime one can identify $\sqrt{\langle \delta N \rangle} / N$ as the small parameter, where $\langle \delta N \rangle \equiv \int d\mathbf{r} \langle \hat{\eta}^\dagger \hat{\eta} \rangle \ll N_C \approx N$. They expand $\hat{\Lambda}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ in powers of $1/\sqrt{N}$:

$$\hat{\Lambda}(\mathbf{r}, t) = \hat{\Lambda}^{(0)}(\mathbf{r}, t) + \frac{1}{\sqrt{N}} \hat{\Lambda}^{(1)}(\mathbf{r}, t) + \frac{1}{N} \hat{\Lambda}^{(2)}(\mathbf{r}, t) + \ldots\quad (2.168)$$

and

$$\phi(\mathbf{r}, t) = \phi^{(0)}(\mathbf{r}, t) + \frac{1}{\sqrt{N}} \phi^{(1)}(\mathbf{r}, t) + \frac{1}{N} \phi^{(2)}(\mathbf{r}, t) + \ldots\quad (2.169)$$

Then, performing the asymptotic expansion in the limit of large $N$ (noting the implicit factor of $\sqrt{N}$ in these expansions, see [25] for more details), they find to various orders of $N^{1/2}$:

**Order $N^{1/2}$: The Gross-Pitaevskii Equation**

Consideration of terms of order $N^{1/2}$ yields the time-dependent Gross-Pitaevskii equation (GPE)

$$\left( -i\hbar \frac{\partial}{\partial t} + \hat{H}_{GP}(\mathbf{r}, t) \right) \phi^{(0)}(\mathbf{r}, t) = \xi(t)\phi^{(0)}(\mathbf{r}, t)\quad (2.170)$$

where the arbitrary real function $\xi(t)$ corresponds to an arbitrary global phase of the wave-function $\phi^{(0)}(\mathbf{r}, t)$. The last term in the one-particle Hamiltonian, $\hat{H}_{GP}(\mathbf{r}, t)$, namely $g_N \left| \phi^{(0)}(\mathbf{r}, t) \right|^2$ describes an effective mean-field potential due to particle interactions. In steady state, the one-body density matrix $\hat{\rho}_1$ is time-independent, and $\phi^{(0)}$ can also be chosen to be time-independent, so the GPE reduces to

$$\hat{H}_{GP}(\mathbf{r}) \left| \phi^{(0)} \right\rangle = \mu \left| \phi^{(0)} \right\rangle$$

where $\xi(t) = \mu$ is a constant determined from the normalisation of $\phi^{(0)}$ to unity. $\mu$, then, represents the lowest-order approximation for the chemical potential of the system. When solving the time-dependent GPE, we usually take the solution of $\hat{H}_{GP}(\mathbf{r}) \left| \phi^{(0)} \right\rangle = \mu \left| \phi^{(0)} \right\rangle$ as the initial condition, with $\xi(t = 0) = \mu$, in particular.

**Order $N^0$: The Time-dependent Bogoliubov-de Gennes Equations**

To order $N^0$, one obtains the equation for the BdGEs

$$i\hbar \frac{\partial}{\partial t} \hat{\Lambda}(\mathbf{r}, t) = \left( \hbar(\mathbf{r}, t) - \xi(t) \right) \hat{\Lambda}(\mathbf{r}, t) + g_N \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) Q(\mathbf{r}', \mathbf{r}'', t) \left| \phi(\mathbf{r}'', t) \right|^2 \hat{\Lambda}(\mathbf{r}'', t)$$

$$+ g_N \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) Q^*(\mathbf{r}', \mathbf{r}'', t) \phi^2(\mathbf{r}'', t) \hat{\Lambda}^\dagger(\mathbf{r}'', t)\quad (2.172)$$

---

7This is the one-particle Gross-Pitaevskii Hamiltonian, and contains both kinetic and potential energy terms.
which can be re-written in operator notation as

\[
\begin{align*}
    i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \hat{\Lambda}(\mathbf{r}, t) \\ \hat{\Lambda}^\dagger(\mathbf{r}, t) \end{bmatrix} &= \hat{L}(t) \circ \begin{bmatrix} \hat{\Lambda}(\mathbf{r}, t) \\ \hat{\Lambda}^\dagger(\mathbf{r}, t) \end{bmatrix} \\
\end{align*}
\]

where

\[
\hat{L}(t) \equiv \begin{bmatrix} \hat{h} + g_N \hat{Q}(t) \phi(\mathbf{r}, t)^2 \hat{Q}(t) - \xi(t) & g_N \hat{Q}(t) \phi^2(\mathbf{r}, t) \hat{Q}(t) \\
- g_N \hat{Q}^*(t) \phi^2(\mathbf{r}, t) \hat{Q}(t) & -\hat{h}^* + g_N \hat{Q}^*(t) |\phi(\mathbf{r}, t)|^2 \hat{Q}^*(t) + \xi(t) \end{bmatrix}
\]

with \(\hat{O} \circ \hat{\Psi} \equiv \int d\mathbf{r}' \hat{O}(|\mathbf{r}'|) \hat{\Psi}(\mathbf{r}')\) and hence \(\hat{O} \circ \hat{\Psi}(\mathbf{r}) \equiv \int d\mathbf{r}' \langle \mathbf{r} | \hat{O} \rangle \hat{\Psi}(\mathbf{r}')\) and where, for example, we note that [65]

\[
\left( \hat{Q}(t) |\phi(\mathbf{r}, t)|^2 \hat{Q}(t) \right) \circ \hat{\Lambda}(\mathbf{r}, t) \equiv \int d\mathbf{r}' \int d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) Q(\mathbf{r}', \mathbf{r}'', t) |\phi(\mathbf{r}'', t)|^2 \hat{\Lambda}(\mathbf{r}'', t).
\]

Order \(\hat{N}^{-1/2}\)- Corrections to the Gross-Pitaevskii Equation To order \(\hat{N}^{-1/2}\) the corrections to the Gross-Pitaevskii equation are zero.

Order \(\hat{N}^{-1}\)- Corrections to the Gross-Pitaevskii Equation To order \(\hat{N}^{-1}\) one finds for the component orthogonal \(\phi^{(2)}_\perp(\mathbf{r}', t)\) to \(\phi^{(0)}(\mathbf{r}', t)\)

\[
- i\hbar \frac{\partial}{\partial t} \phi^{(2)}_\perp(\mathbf{r}, t) = \left( \hat{h}(\mathbf{r}, t) - \xi(t) \right) \phi^{(2)}_\perp(\mathbf{r}, t) + g_N \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) Q(\mathbf{r}', \mathbf{r}'', t) |\phi(\mathbf{r}'', t)|^2 \phi^{(2)}_\perp(\mathbf{r}'', t) \\
+ g_N \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) Q(\mathbf{r}', \mathbf{r}'', t) \phi^2(\mathbf{r}'', t) \phi^{(2)*}_\perp(\mathbf{r}'', t) \\
- g_N \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}', t) \left[ |\phi(\mathbf{r}', t)|^2 \phi(\mathbf{r}', t) \left( 1 + \int d\mathbf{r}''' \bar{n}(\mathbf{r}'', \mathbf{r}'', t) \right) \right] \\
+ g_N \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}', t) \left[ 2\bar{n}(\mathbf{r}', \mathbf{r}', t) \phi(\mathbf{r}', t) + \bar{m}(\mathbf{r}', \mathbf{r}', t) \phi^*(\mathbf{r}', t) \right] \\
- g_N \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) |\phi(\mathbf{r}'', t)|^2 \left[ \bar{n}(\mathbf{r}'', \mathbf{r}', t) \phi(\mathbf{r}'', t) + \bar{m}(\mathbf{r}'', \mathbf{r}', t) \phi^*(\mathbf{r}'', t) \right].
\]

They interpret the above equation as follows:

1. The term \(- g_N \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}', t) \left[ |\phi(\mathbf{r}', t)|^2 \phi(\mathbf{r}', t) \left( 1 + \int d\mathbf{r}''' \bar{n}(\mathbf{r}'', \mathbf{r}'', t) \right) \right] \) corrects the over-estimation of the number of condensed particles in calculating their mutual interactions \(N \to N - \left( 1 + \langle \delta N \rangle \right) \) in the GPE.

2. The term \(g_N \int d\mathbf{r}' Q(\mathbf{r}, \mathbf{r}', t) \left[ 2\bar{n}(\mathbf{r}', \mathbf{r}', t) \phi(\mathbf{r}', t) + \bar{m}(\mathbf{r}', \mathbf{r}', t) \phi^*(\mathbf{r}', t) \right] \) describes the interaction of the condensed particles and the non-condensed ones - we can understand this in terms of the mean-field picture - the Hartree-Fock approximation.

3. The term \(- g_N \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}', t) |\phi(\mathbf{r}'', t)|^2 \left[ \bar{n}(\mathbf{r}'', \mathbf{r}', t) \phi(\mathbf{r}'', t) + \bar{m}(\mathbf{r}'', \mathbf{r}', t) \phi^*(\mathbf{r}'', t) \right] \) corresponds to the spatial correlation of the non-condensed particles.
One can choose the component $\phi^\parallel_2(r, t)$ along $\phi^0(r, t)$ arbitrarily, using the arbitrariness of the global phase of $\phi(r, t)$.

The time-evolution of $\hat{\Lambda}$ They show that the time evolution of the operators $\hat{\Lambda}$ (i.e. the dynamics of the non-condensed particles) amounts to propagating a perturbation orthogonal to $\phi$. They choose a basis which diagonalises $\hat{L}$ at time $t = 0$ given by the Bogoliubov transformation

$$
\hat{\Lambda}(r, t) = \sum_k \left( u_k(r, t)\hat{a}_k + v_k^*(r, t)\hat{a}_k^\dagger \right)
$$

where the usual Bose commutation relations (2.45)

$$
[\hat{a}_k, \hat{a}_l^\dagger] = \delta_{kl} \quad \text{and} \quad [\hat{a}_k, \hat{a}_l] = [\hat{a}_k^\dagger, \hat{a}_l^\dagger] = 0
$$

apply. They show the equivalence of the quantum fluctuations described by $\hat{\Lambda}$ and the time-evolution of small perturbations $\delta \phi$ of the time-dependent solution of the GPE using linear-response theory.

Applicability The formalism of Castin and Dum hasn’t been used as such - Morgan et. al. [60] used linear response theory based on the GGPE (2.84). A systematic expansion approach is used here, so the theory can be extended to higher orders. The order of difficulty is of the same order as that used by Morgan et. al. [60]. The time-dependent formalism, however, is not applicable, because angular momentum conservation is violated - see comments towards bottom of page 89, chapter 4.

The Approach due to S. A. Gardiner et. al.

In their treatment of the time-dependent problem, S. A. Gardiner et. al. [26] follow closely along the lines of the analysis by Castin and Dum [25]. As in [25], they split the Bose field operator $\hat{\psi}(r, t)$ in the Hamiltonian (2.18) subject to the contact potential approximation $U(r) = g\delta(r)$, i.e. Eq. (2.24)

$$
\hat{H}(t) = \int d\mathbf{r} \left( \hat{\psi}^\dagger(r, t)\hat{h}(r)\hat{\psi}(r, t) + \frac{g}{2} \hat{\psi}^\dagger(r, t)\hat{\psi}(r, t)\hat{\psi}(r, t)\hat{\psi}(r, t) \right)
$$

into a condensate part (macroscopic matrix elements), and a non-condensate part (accounting for the remaining non-condensate particles) (2.160)

$$
\hat{\psi}(r, t) = \phi(r, t)\hat{a}_c(t) + \eta(r, t)
$$
where \( \phi(\mathbf{r}, t) \) is normalised to unity. This is justified in the presence of a condensate in view of the fact that there is one distinct eigenfunction \( \phi(\mathbf{r}, t) \) with unit normalisation that has a corresponding eigenvalue \( N_c(t) \) that is much larger than all the other eigenvalues, i.e.

\[
\int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}', t) \phi(\mathbf{r}', t) = N_c(t) \phi(\mathbf{r}, t)
\]

where \( \rho(\mathbf{r}, \mathbf{r}', t) = \langle \hat{\rho}(\mathbf{r}, \mathbf{r}', t) \rangle = \langle \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}', t) \rangle \) is the single-particle density matrix.

They differ in their choice of fluctuation operator from Castin and Dum [25], preferring the choice (c.f. Eq. (2.167))

\[
\hat{\Lambda}(\mathbf{r}, t) = \frac{1}{\sqrt{N_c(t)}} \hat{a}_c^\dagger(t) \hat{\eta}(\mathbf{r}, t)
\]

with commutation relation

\[
\left[ \hat{\Lambda}(\mathbf{r}, t), \hat{\Lambda}^\dagger(\mathbf{r}', t) \right] = \frac{\hat{N}_c(t)}{N_c(t)} Q(\mathbf{r}, \mathbf{r}', t) - \frac{1}{N_c(t)} \hat{\eta}^\dagger(\mathbf{r}', t) \hat{\eta}(\mathbf{r}, t)
\]

where we have defined (2.164)

\[
Q(\mathbf{r}, \mathbf{r}', t) \equiv \delta(\mathbf{r} - \mathbf{r}') - \phi(\mathbf{r}, t) \phi^*(\mathbf{r}', t)
\]

for the following reasons:

1. \( \hat{\Lambda}(\mathbf{r}, t) \) scales as \( \sqrt{N_c(t)} \). The fluctuation operator \( \hat{\Lambda}(\mathbf{r}, t) = \frac{1}{\sqrt{N_c(t)}} \hat{a}_c^\dagger(t) \hat{\eta}(\mathbf{r}, t) \) as used by Castin and Dum [25] scales as \( \sqrt{N_c(t)} N_c(t)/N \approx \sqrt{N_c(t)} \) and therefore scales satisfactorily only when \( N_c(t) \approx N \), hence requiring that the fluctuations are small compared to the square root of the number of condensed particles. The scaling used here, however, is not dependent on the requirement that \( N_c(t) \approx N \).

2. To the order of the calculation used here the commutation relation, \( \left[ \hat{\Lambda}(\mathbf{r}, t), \hat{\Lambda}^\dagger(\mathbf{r}', t) \right] \)

may be taken to be \( Q(\mathbf{r}, \mathbf{r}', t) \).

They note that

\[
\hat{N}_c(t) - N_c(t) = \int d\mathbf{r} \langle \hat{\eta}^\dagger(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) \rangle - \int d\mathbf{r} \hat{\eta}^\dagger(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t)
\]

\[
= \int d\mathbf{r} \langle \hat{\Lambda}^\dagger(\mathbf{r}, t) \frac{N_c(t)}{\hat{N}_c(t)} \hat{\Lambda}(\mathbf{r}, t) \rangle - \int d\mathbf{r} \hat{\Lambda}^\dagger(\mathbf{r}, t) \frac{\hat{N}_c(t)}{N_c(t)} \hat{\Lambda}(\mathbf{r}, t)
\]

\[
\approx \int d\mathbf{r} \langle \hat{\Lambda}^\dagger(\mathbf{r}, t) \hat{\Lambda}(\mathbf{r}, t) \rangle - \int d\mathbf{r} \hat{\Lambda}^\dagger(\mathbf{r}, t) \hat{\Lambda}(\mathbf{r}, t)
\]

to quadratic order in \( \hat{\Lambda}(\mathbf{r}, t) \) (which is sufficient for the level of approximation used here).

Substituting the placement (2.160) and the expression (2.179) for the fluctuation operator
in the Hamiltonian (2.24), and applying the Gaussian approximation of the fluctuation terms

\[ \hat{N}(\mathbf{r}, t)\hat{N}(\mathbf{r}, t) \approx 2 \left\langle \hat{N}(\mathbf{r}, t)\hat{N}(\mathbf{r}, t) \right\rangle \hat{N}(\mathbf{r}, t) + \left\langle \hat{N}(\mathbf{r}, t)\hat{N}(\mathbf{r}, t) \right\rangle \hat{N}(\mathbf{r}, t) \]  

(2.181)

they finally obtain the Hamiltonian \( \hat{H}^{(3)}(t) \) to cubic order (denoted by the superscript (3)) given by

\[ \hat{H}^{(3)}(t) = N_c \hat{H}_0^{(3)}(t) + \sqrt{N} c \hat{H}_1^{(3)}(t) + \hat{H}_2^{(3)}(t) + \frac{1}{\sqrt{N}} \hat{H}_3^{(3)}(t) \]  

(2.182)

where

\[ \hat{H}_0^{(3)}(t) = \int \! d\mathbf{r} \phi^* \left( \hat{h} + \frac{g N_c}{2} |\phi|^2 \right) \phi \]  

(2.183)

\[ \hat{H}_1^{(3)}(t) = \int \! d\mathbf{r} \left[ \phi^* \left( \hat{h} + g N_c |\phi|^2 \right) \hat{\Lambda} + \text{h.c.} \right] \]  

(2.184)

\[ \hat{H}_2^{(3)}(t) = \int \! d\mathbf{r} \left[ \hat{\Lambda}^\dagger \left( \hat{h} + 2 g N_c |\phi|^2 \right) \hat{\Lambda} + \left( \frac{1}{2} g N_c \phi^* \hat{\Lambda}^\dagger \hat{\Lambda} + \text{h.c.} \right) - \frac{1}{2} g N_c |\phi|^4 \right] 
+ \left[ \int \! d\mathbf{r} \left( \left\langle \hat{\Lambda}^\dagger \hat{\Lambda} \right\rangle - \left\langle \hat{\Lambda}^\dagger \hat{\Lambda} \right\rangle \right) \right] \int \! d\mathbf{r} \phi^* \left( \hat{h} + g N_c |\phi|^2 \right) \phi \]  

(2.185)

and

\[ \hat{H}_3^{(3)}(t) = \int \! d\mathbf{r} \left\{ \phi^* \left[ 2 \left\langle \hat{\Lambda}^\dagger \hat{\Lambda} \right\rangle \hat{\Lambda} + \left\langle \hat{\Lambda} \right\rangle \hat{\Lambda}^\dagger \right] + \text{h.c.} \right\} - g N_c \int \! d\mathbf{r} \left[ \phi^* |\phi|^2 \hat{\Lambda} + \text{h.c.} \right] 
+ \int \! d\mathbf{r} d\mathbf{r}' \left\{ \phi^* (\mathbf{r}, t) |\phi(\mathbf{r}, t)|^2 \left\langle \hat{\Lambda}^\dagger(\mathbf{r}', t) \hat{\Lambda}(\mathbf{r}, t) \right\rangle \hat{\Lambda}(\mathbf{r}', t) + \text{h.c.} \right. 
+ \left. \left\langle \hat{\Lambda}(\mathbf{r}', t) \hat{\Lambda}(\mathbf{r}, t) \right\rangle \hat{\Lambda}^\dagger(\mathbf{r}', t) + \text{h.c.} \right\} \} \]  

(2.186)

Then assuming that the bosonic field operator has no explicit time dependence, they obtain to various orders of approximation:

**Order \( N_c^{1/2} \) - The Gross-Pitaevskii Equation**  Considering terms in \( \hat{H}^{(3)}(t) \) to order \( N_c^{1/2} \) (i.e. terms \( \hat{H}_0^{(3)}(t) \) and \( \hat{H}_1^{(3)}(t) \)) yields the time-dependent Gross-Pitaevskii equation

\[ i \hbar \frac{\partial \phi(\mathbf{r}, t)}{\partial t} = \left( \hat{h}(\mathbf{r}, t) + g N_c |\phi(\mathbf{r}, t)|^2 - \lambda_0 \right) \phi(\mathbf{r}, t) \]  

(2.187)

where

\[ \lambda_0 = \int \! d\mathbf{r} \phi^*(\mathbf{r}, t) \left( \hat{h}(\mathbf{r}, t) + g N_c |\phi(\mathbf{r}, t)|^2 - i \hbar \frac{\partial \phi(\mathbf{r}, t)}{\partial t} \right) \phi(\mathbf{r}, t) \]  

(2.188)

(c.f. Castin and Dum [25]) which, in the time-independent case, reduces to

\[ \lambda_0 \phi(\mathbf{r}) = \left( \hat{h}(\mathbf{r}) + g N_c |\phi(\mathbf{r})|^2 \right) \phi(\mathbf{r}) \]  

(2.189)

where \( \lambda_0 \) is an eigenvalue of this equation corresponding to the chemical potential.
Order $Nc^0$ - The Modified Bogoliubov de-Gennes Equations

They find to order $Nc^0$ the generalised BdGEs given by

$$i\hbar \frac{\partial \tilde{\Lambda}(r, t)}{\partial t} = \left( \hat{h} + gNc \left| \phi \right|^2 - \lambda_0 \right) \tilde{\Lambda}(r, t) + gNc \int d\mathbf{r}'Q(r, r', t) \left[ |\phi(r', t)|^2 \tilde{\Lambda}(r', t) + \phi^2(r', t)\tilde{\Lambda}(r', t) \right].$$

(2.190)

Order $Nc^{-1/2}$ - The Generalised Gross-Pitaevskii Equation

They find to order $Nc^{-1/2}$ the GGPE

$$i\hbar \frac{\partial \phi(r, t)}{\partial t} = \left( \hat{h} + gNc \left[ \left( 1 - \frac{1}{Nc} \right) |\phi|^2 + \frac{2}{Nc} \left\langle \tilde{\Lambda}^\dagger \tilde{\Lambda} \right\rangle \right] - \lambda_2 \right) \phi(r, t) + g \left\langle \tilde{\Lambda} \tilde{\Lambda} \right\rangle \phi^*(r, t) - g \int d\mathbf{r}' |\phi(r', t)|^2 \left[ \left\langle \tilde{\Lambda}^\dagger(r', t)\tilde{\Lambda}(r, t) \right\rangle \phi(r', t) + \left\langle \tilde{\Lambda}(r', t)\tilde{\Lambda}(r, t) \right\rangle \phi^*(r', t) \right].$$

(2.191)

The GGPE (2.191) and the modified BdGEs (2.190) describe the second-order coupled condensate and non-condensate dynamics, and constitute the main result of the paper [26].

In the quasi-particle basis, using the Bogoliubov transformation

$$\tilde{\Lambda}(r, t) = \sum_k \left( u_k(r, t)\hat{a}_k + v_k^*(r, t)\hat{a}_k^\dagger \right)$$

(2.192)

the modified BdGEs become

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix} \hat{\mathcal{L}}(r, r', t) & \mathcal{M}(r, r', t) \\ -\mathcal{M}^*(r, r', t) & -\hat{\mathcal{L}}^*(r, r', t) \end{bmatrix} \begin{bmatrix} u_q(r', t) \\ v_q(r', t) \end{bmatrix}$$

(2.193)

where we have defined

$$\hat{\mathcal{L}}(r, r', t) \equiv \delta(r, r') \left( \hat{h}(r) + gNc |\phi(r, t)|^2 - \lambda_0 \right) + gNc \int d\mathbf{r}''Q(r, r'', t)Q(r'', r', t) |\phi(r', t)|^2$$

(2.194)

and

$$\mathcal{M}(r, r', t) \equiv gNc \int d\mathbf{r}''Q(r, r'', t)Q(r'', r', t)\phi^2(r', t)$$

(2.195)

and define the densities

$$\tilde{n}(r', r, t) \equiv \left\langle \tilde{\Lambda}^\dagger(r', t)\tilde{\Lambda}(r, t) \right\rangle, \quad \tilde{n}(r, t) \equiv \left\langle \tilde{\Lambda}^\dagger(r, t)\tilde{\Lambda}(r, t) \right\rangle$$

$$\tilde{m}(r', r, t) \equiv \left\langle \tilde{\Lambda}(r', t)\tilde{\Lambda}(r, t) \right\rangle, \quad \tilde{m}(r, t) \equiv \left\langle \tilde{\Lambda}(r, t)\tilde{\Lambda}(r, t) \right\rangle$$

(2.196)

Here

$$\tilde{n}(r, t) \equiv \left\langle \tilde{\eta}^\dagger(r, t)\tilde{\eta}(r, t) \right\rangle = \sum_q \left[ |u_q(r, t)|^2 N_{BE}(\epsilon_q) + |v_q(r, t)|^2 (N_{BE}(\epsilon_q) + 1) \right]$$
is the thermal density (2.59), and
\[ \tilde{m}(r, t) \equiv \langle \hat{\eta}(r, t)\hat{\eta}(r, t) \rangle = \sum_q u_q(r, t)v_q^*(r, t) \left( 2N_{BE}(\epsilon_q) + 1 \right) \]

the anomalous density (2.60), where \( N_{BE}(\epsilon_q) \) is the Bose distribution for the \( q \)th quasi-particle excitation given by (2.51)
\[ N_{BE}(\epsilon_q) = \frac{1}{\exp(\beta\epsilon_q) - 1} \]

We see that
\[ \tilde{n}(r', r, t) \equiv \langle \hat{\eta}^\dagger(r', t)\hat{\eta}(r, t) \rangle = \sum_q \left[ u_q^*(r', t)u_q(r, t)N_{BE}(\epsilon_q) + v_q(r', t)v_q^*(r, t) \right] \left( N_{BE}(\epsilon_q) + 1 \right) \]
and
\[ \tilde{m}(r', r, t) \equiv \langle \hat{\eta}(r', t)\hat{\eta}(r, t) \rangle = \sum_q \left[ v_q^*(r', t)u_q(r, t)N_{BE}(\epsilon_q) + u_q(r', t)v_q^*(r, t) \right] \left( N_{BE}(\epsilon_q) + 1 \right) \]

The GGPE can then be written
\[ i\hbar \frac{\partial}{\partial t} \phi(r, t) = \left( \hat{h} + gN_c \left[ \left( 1 - \frac{1}{N_c} \right) |\phi|^2 + \frac{2}{N_c}\tilde{n} \right] - \lambda_2 \right) \phi(r, t) + g\tilde{m}\phi^*(r, t) - g \int d r' |\phi(r', t)|^2 \left[ \tilde{n}(r', r, t)\phi(r', t) + \tilde{m}(r', r, t)\phi^*(r', t) \right] . \]

**Problems with this approach** There are various problems associated with this approach:

1. The commutation relation for the fluctuation operator \( \hat{\Lambda} \) given by equation (2.180) is dependent on the fluctuation operator \( \hat{\eta} \). However they neglect this dependency by omitting the last term in (2.180) and by assuming that \( \hat{N}_c/N_c \approx 1 \), thus approximating the commutation relation for the fluctuation operator \( \hat{\Lambda} \) by the quasi-bosonic relation \( \left[ \hat{\Lambda}(r, t), \hat{\Lambda}^\dagger(r', t) \right] \approx Q(r, r', t) \). To quadratic order \( \hat{N}_c(t) - N_c(t) \approx \int d r \left\langle \hat{\Lambda}^\dagger \hat{\Lambda} \right\rangle - \int d r \hat{\Lambda}^\dagger \hat{\Lambda} \), so it is unclear as to how good this approximation really is,

2. They use the Gaussian approximation of the fluctuation terms \( \hat{\Lambda}^\dagger \hat{\Lambda} \approx 2 \left\langle \hat{\Lambda}^\dagger \hat{\Lambda} \right\rangle \hat{\Lambda} + \left\langle \hat{\Lambda} \hat{\Lambda} \right\rangle \hat{\Lambda}^\dagger \), which could raise objections similar to those in the HFB formalism,

3. The reliability of the time-dependent formalism may be questioned because particle, angular and linear momentum conservation are violated since \( \lambda_2 \) is, in general, complex.
2.8 Classical Field Theories

There are several problems associated with mean field theories:

1. The full Hartree-Fock Bogoliubov theory is a conserving theory (i.e. ensures the conservation of physical laws), but introduces an energy gap. The Popov, G1, and G2 theories remedy this, but result in the violation of important physical conservation laws.

2. Number conserving theories ensure that the symmetry is not broken, thereby ensuring number conservation in the absence of approximations, hence one does not have to work in a grand canonical ensemble, thereby avoiding the problems associated with this. Systematic expansions of the Hamiltonian ensure that the energy gap problem is also remedied. However, in endeavouring to ensure the expansion of the Hamiltonian in terms of a small parameter, important physical conservation laws are often violated in time-dependent theories for finite size systems including, ironically, particle conservation. These laws are usually observed in the thermodynamic limit, however.

Here we discuss briefly two methods used in the classical field approach. For further details, the reader is referred to an excellent review article by Blakie et al. [27].

2.8.1 The Projected Gross-Pitaevskii Equation (PGPE) [27, 28]

In the classical field approach we look to describe the modes within a BEC by means of classical fields. The assumption here is that all such modes are highly occupied, an assumption that is only likely to be valid provided the temperatures are not too low. Such methods are very useful in describing quasi-condensates (where the mean-field methods are not generally applicable), and in other areas where the mean-field theories break down.

There are many approaches possible, one of which is the approach due to Davis, Morgan and Burnett [28] wherein the non-linear term $|\phi|^2 \phi$ in the GPE is replaced by $\hat{P} \{ |\phi|^2 \phi \}$, where $\hat{P}$ is the projection operator defined by

$$\hat{P} \{ f(\mathbf{r}, t) \} = \sum_{\mathbf{k} \in \mathcal{C}} \phi_k(\mathbf{r}, t) \int d\mathbf{r}' \phi_k^*(\mathbf{r}', t) f(\mathbf{r}', t) \tag{2.200}$$
for some set of basis functions \(\{\phi_k(r, t)\}\) (usually the single particle basis functions \(\{\xi_k(r)\}\)) for which \(\hat{\psi}(r, t) = \sum_k \hat{a}_k \phi_k(r, t)\). \(k \in C\) means that \(k\) is restricted to the coherent (classical) region \(C\), so the effect of \(\hat{P}\) on the Bose field operator \(\hat{\psi}(r, t)\) given by

\[
\hat{P}\left\{ \hat{\psi}(r, t) \right\} = \sum_{k \in C} \hat{a}_k \phi_k(r, t)
\]  

(2.201)

is to restrict the Bose field operator to the low temperature, coherent regime where the modes are likely to be reasonably heavily occupied, and can therefore be treated as classical fields. The problem then reduces to solving the projected Gross-Pitaevskii equation (PGPE)

\[
i \hbar \frac{\partial \phi(r, t)}{\partial t} = \hat{h}(r, t) \phi(r, t) + g_N \hat{P} \left\{ |\phi(r, t)|^2 \phi(r, t) \right\}
\]  

(2.202)

Assuming we can ignore the quantum fluctuation operator of the projected field operator, we can replace \(\hat{a}_k \rightarrow c_k\), and write \(\hat{\psi}(r, t) = \sum_k c_k \phi_k(r, t)\). Thermal fluctuations are introduced into the treatment\(^8\), and quantities such as condensate fractions and correlation functions need to be averaged over these fluctuations. To do this, one relies on the ergodic hypothesis, and replaces ensemble averages by time averages. The PGPE is useful in the study of non-equilibrium condensation [70, 71], the shift in the critical temperature \(T_c\) [72], and in the study of vortex-antivortex pair production in quasi-2D gases [73], amongst other things.

**Applicability** The PGPE is applicable in the higher temperature regime in situations where many modes are macroscopically occupied in contrast to mean-field theories which are generally valid in the lower temperature regime, and in situations where only one mode (the ground state) is macroscopically occupied. Therefore the PGPE is useful in describing quasi-condensates at temperatures quite near to the transition temperature and other scenario where many states are macroscopically occupied, and as mentioned above, in the study of vortex-anti-vortex production in quasi-2D gases [73], the study of non-equilibrium condensation [70, 71], and in the shift of the critical temperature \(T_c\) [72].

### 2.8.2 Stochastic Methods - The Truncated Wigner Method

We discuss here the truncated Wigner approximation (see for example [27, 29–31], and a very comprehensive discussion in [32]). Here one considers an effective low-energy system by writing the Hamiltonian in terms of the restricted Bose field operator \(\hat{\psi}(r, t) =

\[^8\]Thermal noise can be introduced via stochastic methods (some noise is included in each mode of the classical field \(\psi\)) - see [31, 33–35], for example.
\[ \sum_{i \in C} \langle i | \hat{a}_i | \rangle \] for the basis representation \( \{ |i \rangle \} \). Hence the system may be described by the effective Hamiltonian

\[ \hat{H}_{\text{eff}}(t) = \sum_{i,j \in C} \langle i | \hat{h} | j \rangle \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l \in C} \langle i j | U^{(S)} | k l \rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l. \]  

(2.203)

We are concerned with the evolution of the restricted basis density operator \( \hat{\rho}(t) = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \), which is governed by the von Neumann equation \( i \hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \left[ \hat{H}_{\text{eff}}(t), \hat{\rho}(t) \right] \), thus

\[ i \hbar \frac{\partial \hat{\rho}(t)}{\partial t} = \sum_{i,j \in C} \langle i | \hat{h} | j \rangle \left( \hat{a}_i^\dagger \hat{a}_j \hat{\rho} - \hat{\rho} \hat{a}_i^\dagger \hat{a}_j \right) + \sum_{i,j,k,l \in C} \langle i j | U^{(S)} | k l \rangle \left( \hat{a}_i^\dagger \hat{a}_j \hat{a}_k \hat{a}_l \hat{\rho} - \hat{\rho} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \right). \]  

(2.204)

Using the multi-mode Wigner function [74] for a system of \( M \) modes, defined by

\[ W \{ \alpha_i, \alpha_i^*, i = 1, \ldots, M \} = \frac{1}{\pi^{2M}} \int d\lambda_1^2 \ldots \int d\lambda_M^2 \prod_{i=1}^M \exp \left( -\lambda_i \alpha_i^* + \lambda_i^* \alpha_i \right) \chi_W \]  

(2.205)

where the multimode Wigner characteristic function \( \chi_W \) is defined by

\[ \chi_W \{ \alpha_i, \alpha_i^*, i = 1, \ldots, M \} \equiv Tr \left\{ \hat{\rho}(t) \prod_{i=1}^M \exp \left( -\lambda_i \hat{a}_i^\dagger + \lambda_i^* \hat{a}_i \right) \right\}, \]  

(2.206)

we can then reformulate the von Neumann equation in terms of the Wigner function using the multimode correspondences

\[ \hat{a}_i \hat{\rho}(t) \leftrightarrow (\alpha_i + \frac{1}{2} \partial / \partial \alpha_i^*) W \{ \alpha_i, \alpha_i^*, i = 1, \ldots, M \} \]

\[ \hat{a}_i^\dagger \hat{\rho}(t) \leftrightarrow (\alpha_i^* - \frac{1}{2} \partial / \partial \alpha_i) W \{ \alpha_i, \alpha_i^*, i = 1, \ldots, M \} \]

\[ \hat{\rho}(t) \hat{a}_i \leftrightarrow (\alpha_i - \frac{1}{2} \partial / \partial \alpha_i) W \{ \alpha_i, \alpha_i^*, i = 1, \ldots, M \} \]

\[ \hat{\rho}(t) \hat{a}_i^\dagger \leftrightarrow (\alpha_i^* + \frac{1}{2} \partial / \partial \alpha_i) W \{ \alpha_i, \alpha_i^*, i = 1, \ldots, M \} \].

(2.207)

This yields the third order non-linear differential equation

\[ i \hbar \frac{\partial}{\partial t} W = \sum_{i,j \in C} \langle i | \hat{h} | j \rangle \left( \frac{\partial}{\partial \alpha_i} \alpha_j - \frac{\partial}{\partial \alpha_j} \alpha_i^* \right) W \]

\[ - \sum_{i,j,k,l \in C} \langle i j | U^{(S)} | k l \rangle \left[ \left( \frac{\partial}{\partial \alpha_i} \alpha_l - \frac{\partial}{\partial \alpha_l} \alpha_i^* \right) \left( \frac{\partial}{\partial \alpha_j} \alpha_k - \delta_{jk} \right) \right. \]

\[ - \frac{1}{4} \left( \frac{\partial^3}{\partial \alpha_i \alpha_j \alpha_k} \alpha_l - \frac{\partial^3}{\partial \alpha_j \alpha_k \alpha_i} \alpha_l^* \right) \]  

(2.208)

which is exactly equivalent to the von Neumann equation (2.204), but which is now a classical equation of motion.

As it stands, this problem is soluble in principle, but for large phase space (dimension \( 2M \)) is virtually intractable. However, by truncating the third order terms in the above
equation, we are able to convert between this problem and a set of Fokker-Planck equations. This truncation can be shown to be justified provided \([32]\)

\[
\left| n(r) - \frac{1}{2} \delta_P(r, r') \right| \gg \sum_{i \in C} \frac{\Gamma_i}{4} |\phi_i(r)|^2 \tag{2.209}
\]

where \(\Gamma_i\) are numbers representative of the coherence of state \(i\), and where \(\delta_P(r, r')\) is the restricted delta function defined by \(\delta_P(r, r') \equiv \sum_{i \in C} \phi_i^*(r')\phi_i(r)\), and where \(n(r)\) is the real total particle density, so the truncation is justified in regions where there is high particle density [32]. One thus obtains the truncated Wigner Fokker-Planck equation

\[
i\hbar \frac{\partial W}{\partial t} \approx -\sum_{i \in C} \frac{\partial}{\partial \frac{\alpha_i}{i} \phi_i(r)\alpha_i} \left( \sum_{l \in C} \langle i | \hbar | l \rangle \alpha_l + \sum_{j, k, l \in C} \langle i j | U^{(S)} | kl \rangle \left( \alpha_j^* \alpha_k - \delta_{jk} \right) \alpha_l \right) W
\]

\[
+ \sum_{i \in C} \frac{\partial}{\partial \frac{\alpha_i}{i} \phi_i(r)\alpha_i} \left( \sum_{l \in C} \langle i | \hbar | l \rangle \alpha_l^* + \sum_{j, k, l \in C} \langle i j | U^{(S)} | kl \rangle^* \left( \alpha_j \alpha_k^* - \delta_{jk} \right) \alpha_l \right) W. \tag{2.210}
\]

One then uses the Ito calculus which establishes a correspondence between the Fokker-Planck equation governing the evolution of a multi-mode distribution function \(P(-z, t)\) for variables \(z = (z_1, \ldots, z_i, \ldots)\) given by [75]

\[
\frac{\partial P(z, t)}{\partial t} = -\sum_i \frac{\partial}{\partial z_i} (A_j(z, t) P(z, t)) + \frac{1}{2} \sum_{i, j} \frac{\partial^2}{\partial z_i \partial z_j} \left[ [B(z, t) B^T(z, t)]_{ij} P(z, t) \right] \tag{2.211}
\]

where \(A_j(z, t)\) is the drift vector, and \(B(z, t)\) is the diffusion matrix, and the stochastic differential equation

\[
dz(t) = A(z, t)dt + B(z, t)d\bw(t) \tag{2.212}
\]

where \(d\bw(t)\) is a vector of independent Wiener processes [75] which describes Gaussian random fluctuations around the drift evolution. Thus we can write the stochastic differential equation

\[
i\hbar \frac{d\alpha_i(t)}{dt} = \sum_{k \in C} \langle i | \hbar | k \rangle \alpha_k(t) + \sum_{j, k, l \in C} \langle i j | U^{(S)} | kl \rangle \left( \alpha_j^*(t) \alpha_k(t) - \delta_{jk} \right) \alpha_l(t) \tag{2.213}
\]

for the low energy mode \(\alpha_i(t)\), \(i \in C\), and the complex conjugate equation for the evolution of \(\alpha_i(t)\).

Now it can be shown that, defining the restricted wave-function

\[
\Psi_P(r, t) \equiv \sum_{i \in C} \phi_i(r, t)\alpha_i(t) \tag{2.214}
\]

with conjugate relation

\[
\alpha_i(t) = \int d\r \phi_i^*(r, t) \Psi_P(r, t) \tag{2.215}
\]
for \( i \in C \) that the evolution of the mode amplitudes \( \alpha_i(t) \) may be written as

\[
 i \hbar \frac{\partial \alpha_i(t)}{\partial t} = \int d\mathbf{r} \phi^*(\mathbf{r}, t) \left[ \hat{h}(\mathbf{r}, t) + g_N \left( |\Psi_P(\mathbf{r}, t)|^2 - \delta_P(\mathbf{r}, \mathbf{r}) \right) \right] \Psi_P(\mathbf{r}, t) \tag{2.216}
\]

where we have used the contact potential approximation \( U(\mathbf{r}) = g \delta(\mathbf{r}) \). So by (2.213) and (2.214), we find that

\[
 i \hbar \frac{\partial \Psi_P(\mathbf{r}, t)}{\partial t} = \hat{h}(\mathbf{r}, t) \Psi_P(\mathbf{r}, t) + g_N \mathcal{P} \left\{ \left( |\Psi_P(\mathbf{r}, t)|^2 - \delta_P(\mathbf{r}, \mathbf{r}) \right) \Psi_P(\mathbf{r}, t) \right\}. \tag{2.217}
\]

The term \( \delta_P(\mathbf{r}, \mathbf{r}) \) gives rise to anomalous behaviour in terms of energy conservation, and so therefore needs to be eliminated (the inclusion of this term results in the violation of energy conservation in the presence of any change in the external potential). This finally yields the equation

\[
 i \hbar \frac{\partial \Psi_P(\mathbf{r}, t)}{\partial t} = \hat{h}(\mathbf{r}, t) \Psi_P(\mathbf{r}, t) + g_N \mathcal{P} \left\{ |\Psi_P(\mathbf{r}, t)|^2 \Psi_P(\mathbf{r}, t) \right\} \tag{2.218}
\]

which has the same form as the PGPE (2.202).

**Applicability**  In contrast to the PGPE, the truncated Wigner method is essentially a \( T = 0 \) theory. This follows from the truncation approximation where the third order terms in the Wigner equation (2.208) are ignored, and hence one is restricted to very low energy. *Thermal* noise could potentially be included via stochastic methods - see for example [31, 33–35]. The truncated Wigner approach would be useful in investigating the effects of quantum fluctuations in quasi-condensates at low temperature.

### 2.9 Conclusions

In this chapter we have reviewed the background theory for a dilute Bose gas at extremely low temperatures (below the BEC transition point). Starting with the non-linear Schrödinger equation for the symmetrised many-body wave-function (first quantised form), we introduced the notion of creation and annihilation operators, thereby establishing direct correspondence between the first and second quantised forms. Various approximations for the full second-quantised problem were investigated, namely mean field theory (including symmetry-breaking and number-conserving approaches), classical field theories and the truncated Wigner approach. In chapter 4 we shall investigate more fully the Hartree-Fock-Bogoliubov formalism, and introduce an orthogonalised HFB formalism eliminating some of the shortcomings of the standard HFB theory.
Chapter 3

Vortices in Bose-Einstein Condensates

3.1 Introduction

In this chapter we present a brief survey on vortices in BECs, their stability, and their precession, touching very briefly on solitons. Bose-Einstein Condensates (BECs) are characterised by the macroscopic occupation of some quantum state, usually the ground state (as opposed to Fermions, which obey the Pauli exclusion principle). This occurs at sufficiently low temperatures, and is brought about by the quantum statistical properties of Bosons. Accompanied by this is associated long-range order of the condensate. Thus one can associate with the condensate, an order parameter, which is in this case, the wave function of the quantum state in question. This is manifest in the coherence of the atoms/molecules in the condensate population of the BEC. For a stationary BEC, therefore, the condensate phase is well-defined throughout (apart from topological defects such as vortices which may be present), except in the case of large fluctuations arising in low-dimensional systems at relatively high temperatures. The condensate is supposedly a superfluid, which implies persistent flow, in particular the continued rotation of the fluid in vortices, even when the source of rotation is removed.

Vortices in fluids result from rotation of the fluid at sufficiently high angular frequencies. Classically when a fluid is rotated rapidly, a depletion of the fluid at the centre of rotation results as a consequence of the angular momentum of the fluid due to the rotation. However, when the source of the rotation is removed, the vortex dissipates and the fluid reverts back
to its lowest energy state, which is absence of rotation.

The situation for a BEC is somewhat different. The BEC is described by an order parameter, which is a complex wave function, consisting of an amplitude and a phase. In the ground state, the phase is uniform throughout. The existence of a phase gradient implies flow of the condensate. The velocity flow field is proportional to the gradient of the phase. As a consequence of this, the condensate flow field is irrotational (i.e., the velocity field has curl zero) which implies that vortices, if present, must be quantised. When a phase singularity occurs anywhere within the BEC, this must necessarily be accompanied by zero density of the condensate at that point for the wave function to be well-behaved. Such a phase singularity is known as a topological defect.

Vortices (in two-dimensional systems) and vortex lines (in three-dimensional systems) are examples of topological defects, and would be accompanied by a non-zero quantum winding number $\kappa$ (which, for an axially symmetric trap, coincides with the axial angular momentum quantum number $m$, an eigensate of the axial angular momentum quantum operator $\hat{L}_z$). In a two-dimensional or three-dimensional BEC, a phase singularity would imply a circular phase gradient, resulting in a velocity field circulating about the singularity, so the condensate would tend to flow about this point, resulting in a vortex. There also exists a region centred on the singularity, called the core of the vortex, where the wave function amplitude steadily increases as one moves further away from the centre of the core. The core radius would be roughly that radius at which the amplitude of the wave function matches the amplitude of the bulk of the condensate. The classical analogue of this would be a whirlpool. The significant difference is, however, that the flow of a superfluid is irrotational, which rules out, for example, solid body rotation for a single vortex. We can see this if we consider the example of a BEC in an axially symmetric trap, with a vortex centered on the axis. A stable normal density mode in this configuration is possible only if the condensate density is proportional to $e^{i m \phi}$, where $m$ is some integer, and $\phi$ is the angle of rotation about the axis. We see that the vortex is quantised with angular quantum number $m$, which coincides with the winding quantum number $\kappa$, as pointed out earlier.

In the absence of any topological defects, $\kappa = 0$ and the macroscopically occupied quantum state is the ground state with uniform phase. So, for the case of our axially symmetric system, the BEC in the absence of vortices would be characterised by $m = 0$. It turns out that vortices having $|m| > 1$ are in general unstable (see, for example [79]), since it would be energetically more favourable for a multi-charged vortex to break up into singly-charged vortices. So stable vortices would then be characterised by $m = \pm 1$, where $m = 1$
corresponds to a clockwise rotating vortex, and $m = -1$, an anticlockwise rotating vortex.

In one-dimensional systems, one can impose a phase singularity at a given point, by phase imprinting, for example. This would be an example of a topological defect in one dimension. One would expect a topological defect of this type to be the one-dimensional analogue of the vortex in a two-dimensional system. An example of such a topological defect is a dark soliton in a 1D BEC with repulsive interactions having velocity zero \[8, 76–78\]. Such a soliton has a discontinuity in the phase of $\pi$ at the point of the soliton, and may therefore be regarded as a 1D topological defect. Solitons (also known as solitary waves) are localised disturbances which propagate without change of form \[8\]. This is made possible in BECs due to the non-linearity of the GPE, where exact solutions can be found in 1D for homogeneous systems. The subject of solitons is vast (see for example \[8, 76–78\]), and will not be presented in this thesis where we shall concentrate more on vortices in quasi-2D BECs.

### 3.2 The Theory of Vortices in Bose-Einstein Condensates

The flow in superfluids is dissipationless, so we would expect the rotation associated with a vortex to be persistent when the source of rotation is removed. It is interesting, therefore, to investigate whether the theory of BECs leads to this conclusion. The conclusion of the theory would also need to be tested against experiment.

Much of the earlier theoretical work on the dynamics of vortices (see for example \[36–39, 79\]) assumed $T = 0$ and neglected the effects of the non-condensate dynamics on the overall dynamics of the vortex. The stability of vortices is of paramount concern for, as we pointed out earlier, the persistence of vortices in the absence of the source of rotation is an important property of superfluids. Rokshar’s work \[79\] was very important in that it showed that when the non-condensate dynamics is ignored, a vortex in a harmonic trap is never locally stable. Rokshar argues that in view of the existence of a state of lower energy than the condensate state with angular momentum quantum $m$ (which he calls the core state, which as we shall see later is just the anomalous mode), that it would be energetically favourable for particles to be transferred from the condensate vortex state to the core state. This results in the existence of two co-existing condensate states. The resulting many-body ground state may then be described by the superposition of the vortex condensate state.
and the core state \[79\]
\[
\Phi = \sqrt{1-x_{core}}\Phi_m + e^{i\chi}\sqrt{x_{core}}\Phi_{core}
\]  
where \(x_{core} = N_{core}/N\), \(N_{core}\) is the number of atoms in the core state, and \(N\) is the total number of atoms.

If the vortex axis is along the z-axis, and the phase angle \(\chi\) is assumed to be zero (which can be done without loss of generality), the wave functions \(\Phi_m\) and \(\Phi_{core}\) interfere destructively off the y-axis and for \(x > 0\). It follows that the vortex core moves off-axis in the x-direction. Thus Rokshar concludes that the on-centre state can be stable only if the vortex core is pinned to the centre of the trap by a locally repulsive potential. Rokshar shows that the variation in energy due to small variations of the axially symmetric vortex wave function \(\psi = \psi_m + \delta\psi\) is always negative and that therefore the axially symmetric state \(\psi_m\) is not a local minimum of the energy functional

\[
\frac{E}{N} = \int d^3r \psi^* \left( \hat{h} + \frac{g}{2} |\psi|^2 \right) \psi
\]

subject to the constraint that \(\psi_m \sim e^{im\phi}\) where (2.22)

\[
\hat{h}(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V_T(\mathbf{r})
\]

and that therefore the on-axis vortex is unstable. Rokshar [79] (see also [80]) shows that the instability results in a displacement of the vortex, and that Ehrenfest’s theorem implies precession accompanied by dissipation of the vortex.

Fetter [37] has shown analytically using the GPE for the cases of a rotating uniform fluid and for a non-uniform rotating fluid with a Thomas-Fermi (TF) profile density \(n = n(0) \left( 1 - \frac{\rho^2}{R^2} \right)\) for a vortex on the axis of an axially symmetric system, that there exists critical rotational frequencies \(\Omega_0\) and \(\Omega_{CI}\) such that the vortex is in a true equilibrium state when the rotational frequency of the fluid \(\Omega \geq \Omega_{CI}\) (corresponding to the flow velocity exceeding the Landau critical velocity \(v_{LC}\) given by the local speed of sound), and metastable for \(\Omega_0 < \Omega < \Omega_{CI}\). For \(\Omega < \Omega_0\), Fetter shows that the free energy decreases monotonically with increasing \(x\) (distance from axis), so that the vortex spirals outwards and annihilates with its image vortex (which resides on the boundary of the BEC).

He shows that for \(\Omega > \Omega_0\), the free energy increases monotonically with increasing \(x\), consequently if the vortex is displaced slightly (but not too much) from the axis, it tends to return to the axis.

For \(\Omega \geq \Omega_{CI}\), the vortex is always stable, and returns to the axis regardless of how large the displacement.
In a later paper Svidzinsky and Fetter [38] show that a vortex in a trapped BEC has a mode (the anomalous mode) of positive norm and negative energy (and hence frequency). This result is for $T = 0$ and ignores the non-condensate dynamics. This mode is formally unstable in view of its negative energy. He shows that the negative frequency of the mode corresponds to the precession of the vortex around the axis of symmetry of the trap, and that the solution becomes stable above an angular velocity $\Omega_0$, characterising the onset of metastability, (ie. stability with respect to small radial displacements from the central axis).

Dodd et. al. [39] solved the time independent Bogoliubov equations ($T = 0$, ignoring noncondensate dynamics) and found the existence of an eigenvalue having an energy lower than that of the vortex state $\Phi_m(r)$ (ie. negative energy) implying the instability of the solution to the Bogoliubov equations for a condensate containing a singly quantised vortex on the axis. This is identified by Fetter [37] as the so-called anomalous mode. How this comes about is as follows:

The physical solutions to the BdGEs (2.50) must be consistent with the Bose commutation relations, which necessitates the normalisation condition (2.54)

$$\int dr \left( |u_q(r, t)|^2 - |v_q(r, t)|^2 \right) = 1. \tag{3.3}$$

Consequently only positive norm solutions are physical, ie. those for which

$$\int dr \left( |u_q(r, t)|^2 - |v_q(r, t)|^2 \right) > 0.$$

In solving the BdGEs, half the solutions have positive norm, and half negative norm, so we choose the physical positive norm solutions. When solving the BdGEs for a BEC in the absence of vortices, all the energies corresponding to the positive norm solutions are positive (and those corresponding to the negative norm solutions are negative). The unstable mode that Dodd et. al. [39] found for the singly charged vortex on axis ($m = 1$) corresponds to the lowest energy positive norm solution for the quasi-particle energies, and the energy corresponding to this mode is negative. This is known as the anomalous mode.

Interestingly, the work by Dodd et. al. [39] was originally inspired by the quest for a method of identifying vortices in an experiment. The method of detection of vortices by current imaging techniques suffers from the constraint that the viewing of the condensate must be done in a direction roughly perpendicular to the trap axis. This is due to the magnet geometries used. Most imaging setups require images of the condensate densities integrated along the line of sight (as one would logically expect). Clearly it would be desirable to
integrate the density in the plane perpendicular to the trap symmetry axis (also taken to be the axis of rotation) in order to identify the vortex, but instead the acquired image is along this plane, so it is difficult to distinguish between a vortex state and the condensed ground state in this plane. Dodd et. al. [39] showed that the excitation spectrum corresponding to the vortex state would be quite different to that of the ground state, and hence the excitation spectroscopy of the vortex line could be used to identify vortices.

Garcia-Ripoll and Perez-Garcia [83] also studied (in 1999) the stability of axially symmetric vortices in trapped gases subject to rotation. They solved the GPE and BdGEs in the Bogoliubov approximation for a three-dimensional condensate in both the cases of spherically and cylindrically symmetric traps. Their calculations were done for a wide range of non-linearity constants of the GPE, ranging from very small values to very large values. They investigated the stability of vortices for the case of the $m = 1$ and $m = 2$ vortex states, and found that vortices are always energetically unstable for non-rotating systems, but in the case of the vortex state with $m = 1$, the vortex can be stabilised by rotation above a certain critical frequency of rotation, in agreement with the work of Rokshar [79] and of Fetter et. al. [40]. They found that multi-charged vortices ($m = 2$ and higher) can never be energetically stable (a local minimum of the energy functional), and conclude that the absolute minimum of the energy is not an eigenstate of the $\hat{L}_z$ operator, even when the angular frequency of rotation exceeds the critical rotational frequency.

They point out that when a system is unstable in the sense that the BdGEs are unstable, i.e. linear dynamical instability of the linearised system (LS), it is impossible for the system to be stable in the Lyapunov sense, i.e. Lyapunov dynamical stability (LDS) or in the sense of energetic stability (ES), since

$$\text{ES} \Rightarrow \text{LDS} \Rightarrow \text{LS}$$

and so consequently

$$\overline{\text{LS}} \Rightarrow \overline{\text{LDS}} \Rightarrow \overline{\text{ES}}$$

As we have seen above, all analyses neglecting the dynamics of the non-condensate led to the conclusion that below a critical rotational frequency these vortices were unstable and precessed, dissipating out of the condensate.

In 1999 Isoshima et. al. [2] examined the stabilization of vortices confined by a harmonic potential by the effect of the non-condensate at finite temperatures, or alternatively, by an additional pinning potential (eg. a potential produced by a laser beam focussed at the vortex centre). They solve the time-independent modified GPE (2.81) and BdGEs (2.82)
in the Popov approximation. We have seen that solving the GPE and the BdGEs in the Bogoliubov approximation gives us a negative energy for the lowest core localised state (LCLS) (ie. the lowest energy mode, the anomalous mode). Clearly applying the above to finite temperatures yields a divergent Bose distribution giving divergent solutions to the BdGEs. In this case, the solutions to the BdGEs are meaningless. One needs to include the non-condensate density for finite temperature solutions.

The authors consider an axially symmetric system where the wavefunctions vanish at radius \( r = R \) and apply periodic boundary conditions along the \( z \)-axis of period \( L \). They consider a vortex line passing through the centre of the cylinder, and express the condensate wavefunction \( \Phi(\mathbf{r}) \) as

\[
\Phi(r, \theta, z) = \phi(r) e^{im\theta}
\]

and write the quasiparticle amplitude \( u_q(\mathbf{r}) \) and \( v_q(\mathbf{r}) \) as

\[
\begin{align*}
    u_q(\mathbf{r}) &= u_q(r) e^{i\frac{2\pi}{L} q_z z} e^{i(q_\theta + m)\theta} \\
    v_q(\mathbf{r}) &= v_q(r) e^{i\frac{2\pi}{L} q_z z} e^{i(q_\theta - m)\theta}
\end{align*}
\]

where \( \mathbf{q} = (q_r, q_\theta, q_z) \) represents the radial, angular and axial quantum numbers

\[
\begin{align*}
    q_r &= 1, 2, 3, \ldots \\
    q_\theta &= 0, \pm 1, \pm 2, \ldots \\
    q_z &= 0, \pm 1, \pm 2, \ldots
\end{align*}
\]

They expand the quasiparticle amplitudes \( u_q(\mathbf{r}) \) and \( v_q(\mathbf{r}) \) in terms of the eigenfunctions \( \phi^{(i)}_\nu(\mathbf{r}) \)

\[
\begin{align*}
    u_q(\mathbf{r}) &= \sum_i c_q^{(i)} \phi^{(i)}_{q_\theta + m}(\mathbf{r}) \\
    v_q(\mathbf{r}) &= \sum_i d_q^{(i)} \phi^{(i)}_{q_\theta - m}(\mathbf{r})
\end{align*}
\]

according to the method of Gygi and Schluter [84] where the eigenfunctions are given in terms of Bessel functions, and substituting (3.7) into the BdGEs (2.82) and applying the orthogonality properties of the eigenfunctions \( \phi^{(i)}_\nu(\mathbf{r}) \) they obtain a matrix equation for the coefficients \( c_q^{(i)} \) and \( d_q^{(i)} \) of the form

\[
\begin{bmatrix}
    A(q_\theta + m, q_z) & B(q_\theta, m) \\
    -B^T(q_\theta, m) & -A(q_\theta - m, q_z)
\end{bmatrix}
\begin{bmatrix}
    c_q \\
    d_q
\end{bmatrix}
= \epsilon_q
\begin{bmatrix}
    c_q \\
    d_q
\end{bmatrix}
\]

where

\[
A_{ij}(q_\theta \pm m, q_z) = \frac{\hbar^2}{2m} \left( \left( \alpha^{(i)}_\nu \right)^2 + q_z^2 \right) \delta_{i,j} - \mu \delta_{i,j} + \int_0^R (V + 2g (\phi^2 + \mathbf{n})) \phi^{(i)}_{q_\theta \pm m} \phi^{(j)}_{q_\theta \pm m} r dr,
\]

(3.9)
\[ B_{ij} (q_\theta, m) = \int_0^R g \phi^2 \phi^{(i)}_{q_\theta+m} \phi^{(i)}_{q_\theta-m} r dr, \]  

\[ A (q_\theta \pm m, q_z) = \begin{bmatrix} A_{11} (q_\theta \pm m, q_z) & A_{12} (q_\theta \pm m, q_z) & \ldots \\ A_{21} (q_\theta \pm m, q_z) & A_{22} (q_\theta \pm m, q_z) & \ldots \\
\vdots & \vdots & \ddots \end{bmatrix}, \]  

\[ B (q_\theta, m) = \begin{bmatrix} B_{11} (q_\theta, m) & B_{12} (q_\theta, m) & \ldots \\ B_{21} (q_\theta, m) & B_{22} (q_\theta, m) & \ldots \\
\vdots & \vdots & \ddots \end{bmatrix}, \]  

\[ \mathbf{c}_q = \begin{bmatrix} c^{(1)}_q \\ c^{(2)}_q \\ \vdots \end{bmatrix}, \quad \mathbf{d}_q = \begin{bmatrix} d^{(1)}_q \\ d^{(2)}_q \\ \vdots \end{bmatrix}, \]  

and \( \alpha^{(i)}_{\nu} \) is the \( i^{th} \) zero of \( j_{\nu}(r) \), the Bessel function of order \( \nu \).

It can be shown (see comment in [2], and reference [41]) that the eigenvalues of the BdGEs (2.82) and hence of equation (3.8) are real and will then lead to meaningful results. Solving (3.8) yields the coefficients \( \mathbf{c}_q^{(i)} \), \( \mathbf{d}_q^{(i)} \) in the expansion for the quasiparticle amplitudes and the eigenvalues for the BdGEs (3.8), hence a solution can be found. Solving the GGPE (2.81) and the BdGEs (2.82) they find the LCLS to be positive and explain the solution of this mode in terms of the condensate and non-condensate density profiles as calculated in the following way:

The condensate density at the centre of the vortex remains zero, but the non-condensate density is peaked at the centre. The non-condensate density tends to push out the condensate from the centre (since the interactions are repulsive). If the non-condensate density is sufficient, this stabilises the vortex.

We can also think of this in terms of the effective potential [2]

\[ V_{\text{eff}}(r) = V(r) + 2g \left( |\phi(r)|^2 + \bar{n}(r) \right) \]  

which acts as an effective pinning potential that prevents the vortex from moving outward. This stabilisation due to the non-condensate is possible even at \( T = 0 \) provided there is a sufficient thermal population to stabilise the vortex.

This work by Isoshima et. al. was followed up about a year later by Virtanen, Simula and Salomaa [3], where again the generalised GPE and the BdGEs are solved to yield a positive lowest energy mode, in agreement with Isoshima [2]. However, in addition to performing these calculations in the Popov approximation, as was the case in the work by Isoshima et. al.
al., they also performed these calculations using the G1 and G2 gapless mean-field approximations (equations (2.74) and (2.75)) which take into account the effects of scattering of the thermal gas off the condensate (which are neglected in the Popov approximation [5,11]), thus the dynamics of the condensate and non-condensate are treated on a more equal footing. They perform the calculations for the same physical parameter values for the gas and the trap as used by Isoshima et. al. [2] and obtain similar results for the mode energies, and the condensate and non-condensate densities for the Popov, G1 and G2 approximations. They thus predict the local stability of the vortex in these approximations as opposed to the instability predicted by the Bogoliubov approximation [37, 39, 40, 79]. They conclude from this (as do Isoshima et. al. [2]) that the thermal gas is concentrated in the vortex core, thus filling the space left by the condensate. It exerts outward pressure on the condensate, preventing it from collapsing into the core, thus stabilising the vortex. The fact that the LCLS is positive shows that the vortex is locally energetically stable in a non-rotating system, even in the zero-temperature limit. The authors also point out that the fact that the energy of the LCLS is positive implies that vortices displaced slightly from the symmetry axis of the trap precess in the opposite direction of condensate flow about the core. This is in contradiction to experiments\(^1\) performed around that time (2000) which show that the precession of the vortex occurs in the same direction as the core, with the exception of a few “rogue” vortices [85], which implies a negative LCLS energy as predicted by the zero-temperature Bogoliubov approximation. They argue that this discrepancy could be due to an insufficient thermal density in the region of the moving vortex core in the experiments performed.

The calculations performed by Isoshima et. al. [2] and Virtanen et. al. [3] show that when one takes into consideration the dynamics of the non-condensate, stable solutions do exist for singly charged vortices \(|m| = 1\) provided that the core of the vortex contains a sufficiently large density of thermal atoms. Both sets of calculations assume a vortex on the trap axis, but neither indicate the consequences of the vortex being displaced from the axis.

In a later paper in 2002, Virtanen et. al. [86] consider the case of an off-axis vortex in the

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\(^1\)This also seems unreasonable since the GPE prediction is for precession of vortices to occur in the same direction of the condensate flow about the core. One would reasonably expect a continuous change in the precessional frequency of vortices with increasing temperature, and not a discontinuity as this seems to indicate. Our calculations for off-axis vortices (see later) indeed reveal that this is the case, and that the precessional frequencies and the LCLS energies are uncorrelated. Later work by Isoshima et. al. [4] concludes that the precessional frequencies and LCLS energies are uncorrelated, in agreement with the findings here.
Popov approximation. In order to obtain stationary solutions to the generalised GPE and the BdGEs, it is necessary to perform these calculations in the rotating frame. Assuming the frame to be rotating about the trap axis with angular velocity $\Omega$, the single-particle Hamiltonian (for the time-dependent formulation) is given by (equations (2.22) and (2.25))

$$\hat{h}_\Omega(r, t) = \hat{h}(r) - \Omega \cdot \mathbf{L} \tag{3.15}$$

where the angular momentum operator is defined $\mathbf{L} \equiv i\hbar (\mathbf{r} \times \nabla)$.

They consider a repulsively interacting BEC ($g > 0$) containing a precessing vortex line for a gas trapped by a static, axi-symmetric potential, and assume for simplicity, that the vortex moves in a circular orbit about the trap symmetry axis at a constant angular velocity $\Omega$. This is a reasonable assumption since such precessional motion has been observed in the experiments.

They assume the system to contain a sufficient thermal density such that the quasiparticle normal and anomalous distribution functions $\langle \hat{\eta}^\dagger(r, t)\hat{\eta}(r, t) \rangle$ and $\langle \hat{\eta}(r, t)\hat{\eta}(r, t) \rangle$ are constant in time and argue that the mean-field Hamiltonian is then time-independent in the rotating frame.

They note that the thermal density and energetic stability of the system are determined by the quasi-particle (QP) excitation spectrum in the laboratory frame (LF) (ie. the non-rotating frame), and that there is a relationship between the expectation values of the QP energies in the LF (note the QP energies in the LF are not stationary), so it is only meaningful to speak of the expectation values of the QP energies in the LF given by

$$\langle \epsilon_q \rangle = \epsilon'_q + \Omega \cdot \langle l \rangle \tag{3.16}$$

This follows from the form of the Hamiltonian, equation (2.24) in the rotating frame, with the single particle Bose Hamiltonian given by equation (2.25).

They find a relationship for the expectation value of the energy eigenvalue in the LF in terms of the QP amplitudes and condensate wavefunction given by

$$\langle \epsilon_q \rangle = \int d\mathbf{r} \left( u_{q}^*\hat{L}u_{q} + v_{q}^*\hat{L}v_{q} - g\Phi^2u_{q}^*v_{q} - g\Phi^*\Phi u_{q}v_{q}^* \right) \tag{3.17}$$

The operators $\hat{L}$ and $\hat{L}_\Omega$ are related by

$$\hat{L}_\Omega = \hat{L} - \Omega \cdot \mathbf{L} \tag{3.18}$$

where $\hat{L}_\Omega = \hat{h}_\Omega(r) - \mu + 2g(n_c(r, t) + \bar{n}(r, t))$ is the operator for the rotating frame, and $\hat{L} = \hat{h}(r) - \mu + 2g(n_c(r, t) + \bar{n}(r, t))$ the operator corresponding to the LF.
They establish a lower bound for $\langle \epsilon_q \rangle$ using the Thomas-Fermi (TF) approximation, resulting in the expression

$$\langle \epsilon_q \rangle = \int_C d\mathbf{r} \rho \left( V_{tr} + 2g\bar{n} - \mu \right) - g \max \left\{ n_c^{(TF)} - n_c \right\} \int_{C'} d\mathbf{r} \rho$$  \hspace{1cm} (3.19)

where $C$ represents the core region, and $C'$ the region outside the core, $n_c^{(TF)}$ is the TF approximation for the condensate density, $V_{tr}$ is the trapping potential, and $\rho(\mathbf{r})$ is the QP density given by

$$\rho(\mathbf{r}) = \sum_q \left( |u_q(\mathbf{r})|^2 + |v_q(\mathbf{r})|^2 \right)$$  \hspace{1cm} (3.20)

Defining

$$w = \frac{\int_C d\mathbf{r} \rho(\mathbf{r})}{\int_{C'} d\mathbf{r} \rho(\mathbf{r})}$$  \hspace{1cm} (3.21)

they obtain finally a lower bound for the QP energy in the LF, given by

$$\langle \epsilon_q \rangle = \int_C d\mathbf{r} \rho \left( V_{tr} + 2g\bar{n} - \mu - \frac{g \max_{C'} \left\{ n_c^{(TF)} - n_c \right\}}{w} \right)$$  \hspace{1cm} (3.22)

They note that $\bar{n}(\mathbf{r}) \lesssim \frac{1}{2} n_0(\mathbf{r})$ for some $\mathbf{r}$ lying within the core when $Na_s/a_{h0} \gtrsim 1$, see reference [86], where $a_s$ is the s-wave scattering length, $a_{h0}$ is the harmonic oscillator length given by $a_{h0} = \sqrt{\hbar/m\bar{\omega}}$, and $\bar{\omega}$ is the geometric mean of the harmonic oscillator frequency given by $\bar{\omega} = \sqrt{\omega_x \omega_y \omega_z}$. This is valid in the region of interest. They conclude that the anomalous energies become positive for non-condensate in the core filling approximately half the core volume. These predictions are true in the Popov approximation, but they argue that it is straightforward to generalise to the G1 and G2 approximations.

In this way the authors show that the presence of a sufficiently large thermal density provides an effective potential which stabilises the off-axis vortex (as was concluded earlier for the on-axis vortex [2, 3]). The conclusions are the same whether the vortex is on-axis or off-axis. In both cases the non-condensate component prevents the collapse of the vortex by its repulsive action on the condensate, acting as an effective pinning potential for the vortex, as pointed out in their earlier paper [3] (see also [86])). We shall, however, demonstrate in chapter 7 that this is not the case, but that the vortex is stable provided sufficient angular momentum is present in the BEC, below which vortices cannot exist in regions of finite density. In chapter 7 we obtain predictions for the precessional frequency by solving the orthogonal HFB equations self-consistently with the continuity equation for the condensate density in the frame rotating at the precessional frequency (see section 4.2.7 in chapter 4). These results are consistent with the $T = 0$ (Bogoliubov) case where the excitation energy.
of the anomalous mode is zero in the rotating frame. The picture presented in [2, 3] is inconsistent with the $T = 0$ (Bogoliubov) case, and is therefore physically unreasonable.

3.3 Conclusions

In this chapter we presented a brief survey on vortices in BECs, their stability, and their precession, touching very briefly on solitons. We saw in the $T = 0$ case, where the non-condensate dynamics is ignored, that a vortex in a trapped BEC has a mode (the anomalous mode) of positive norm and negative energy (and hence frequency). This mode is formally unstable in view of its negative energy, but becomes stable above an angular velocity $\Omega_0$, characterising the onset of metastability, (ie. stability with respect to small radial displacements from the central axis) and stable above an angular velocity $\Omega_{Cl}$ corresponding to the flow velocity exceeding the Landau critical velocity. In the finite temperature case, the calculations performed by Isoshima et. al. [2] and Virtanen et. al. [3] for on-axis vortices, and generalised to off-axis vortices by Virtanen et. al. [86], show that when one takes into consideration the dynamics of the non-condensate, stable solutions do exist for singly charged vortices ($|m| = 1$) provided that the core of the vortex contains a sufficiently large density of thermal atoms. They attributed the LCLS energy to the precessional frequency of the vortex, leading one to the erroneous conclusion that the vortex precesses in the opposite direction of condensate flow about the core. This is in contradiction to experiments performed around that time (2000) which show that the precession of the vortex occurs in the same direction as the core which implies a negative LCLS energy as predicted by the zero-temperature Bogoliubov approximation. One would reasonably expect a continuous change in the precessional frequency of vortices with increasing temperature, and not a discontinuity as this seems to indicate. Our calculations for off-axis vortices in chapter 7 reveal that this is indeed the case, and that the precessional frequencies and the LCLS energies are uncorrelated. Later work by Isoshima et. al. [4] concludes that the precessional frequencies and LCLS energies are uncorrelated, in agreement with the findings here.

In the next chapter, we shall investigate more fully the Hartree-Fock-Bogoliubov formalism, and introduce an orthogonalised HFB formalism eliminating some of the short-commings of this theory. Conservation laws are investigated, and the continuity equation for the condensate density used to predict the precessional frequencies of off-axis vortices in BECs. These calculations are performed in chapter 7 for BECs having single off-axis vortices and for vortex arrays.
Chapter 4

Development of the Hartree-Fock-Bogoliubov Method

4.1 Introduction

In chapter 2 we discussed the second-quantised Bose Hamiltonian, and its direct correspondence with the first quantised form. We also discussed at length various methods of approximating the full quantum treatment of the many-body problem for a system of Bosons, in particular mean-field theories both symmetry-breaking and number-conserving, and two classical field approaches, i.e. the projected Gross-Pitaevskii equation (PGPE) and the truncated Wigner approach. In this chapter we shall be focussing more on the Hartree-Fock-Bogoliubov (HFB) formalism. In particular, we shall be discussing conservation laws with reference to conservation of particle number, energy, linear momentum, and angular momentum. We apply the continuity equation for the condensate density in predicting the precessional frequencies of vortices in pseudo-two-dimensional BEC systems. Later in section 4.3, we shall develop an orthogonal HFB formalism which addresses some of the problems associated with standard HFB.

We opt here for a mean-field approximation and symmetry-breaking approach, leading to the Hartree-Fock-Bogoliubov formalism. We motivate this on the grounds that these equations can also be derived from a variational standpoint. We shall also see in Chapter 5 that the time-dependent formalism predicts the Kohn mode exactly, in spite of the energy gap problems associated with time-independent HFB, and the violation of the Hugenholtz-Pines theorem requiring the existence of a Goldstone mode. In our development of an
orthogonal form of the HFB theory, we demonstrate that it does at least have a zero-energy excitation. Furthermore, the orthogonal theory satisfies all the conservation laws. Consideration of the perturbation Hamiltonian $\Delta \hat{H}_{13} + \Delta \hat{H}_{24}$ in (4.43) reveals a correspondence to leading second order with the perturbation Hamiltonian in S. A. Morgan’s treatment [23, 24] in equation (2.139). Hence we are able to establish a gapless orthogonal HFB formalism where the quasi-particle energy shifts are calculated self-consistently using equation (2.151) and the orthogonalised HFB equations.

4.2 The Hartree-Fock-Bogoliubov Formalism

4.2.1 The Time-dependent Hartree-Fock-Bogoliubov Equations

Previously we considered the Grand-Canonical Bose Hamiltonian (2.32). In the contact potential approximation $U(r - r') = g\delta(r - r')$, where $g$ is given by (2.23), the Grand-Canonical Bose Hamiltonian may now be written

$$\hat{H}^{(GC)}(t) = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}, t) \left( \hat{h}(\mathbf{r}) - \mu \right) \hat{\psi}(\mathbf{r}, t) + \frac{g}{2} \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t)$$

(4.1)

where (2.22)

$$\hat{h}(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V_T(\mathbf{r})$$

(4.2)

is the single-particle Hamiltonian for an atom confined by a trapping potential $V_T(\mathbf{r})$. As we have seen, the inclusion of the chemical potential $\mu$ ensures that the total number of particles is fixed. We confirm shortly in section (4.2.5) that this is the case, and that the other conservation laws are also observed, but first let us return to the time-dependent HFB equations. In chapter 2 we followed the spontaneous symmetry-breaking approach, writing $\hat{\psi}(\mathbf{r}, t) = \Phi(\mathbf{r}, t) + \hat{\eta}(\mathbf{r}, t)$ (2.30) for the Bose field operator. Hence we derived the Hartree-Fock-Bogoliubov (HFB) (equations (2.62) and (2.63)), consisting of the Generalised Gross Piteavskii equation (GGPE)

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left( \hat{h}(\mathbf{r}) - \mu + g(\Phi(\mathbf{r}, t))^2 + 2\bar{n}(\mathbf{r}, t) \right) \Phi(\mathbf{r}, t) + g\bar{n}(\mathbf{r}, t)\Phi^*(\mathbf{r}, t)$$

(4.3)

and the Bogoliubov de Gennes Equations (BdGEs)

$$i\hbar \frac{\partial}{\partial \tau} \begin{bmatrix} u_q(\mathbf{r}, t) \\ v_q(\mathbf{r}, t) \end{bmatrix} = \begin{bmatrix} \hat{L}(\mathbf{r}, t) & \mathcal{M}(\mathbf{r}, t) \\ -\mathcal{M}^*(\mathbf{r}, t) & -\hat{L}^*(\mathbf{r}, t) \end{bmatrix} \begin{bmatrix} u_q(\mathbf{r}, t) \\ v_q(\mathbf{r}, t) \end{bmatrix}$$

(4.4)
where we defined

\begin{align}
\hat{L}(r, t) &\equiv \hat{h}(r) - \mu + 2g \left(|\Phi(r, t)|^2 + \tilde{n}(r, t)\right) \\
\mathcal{M}(r, t) &\equiv g \left(\Phi^2(r, t) + \tilde{m}(r, t)\right)
\end{align}

(4.5)

with the thermal (2.59), and anomalous (2.60) densities given respectively by

\[\tilde{n}(r, t) \equiv \langle \hat{\eta}^\dagger(r, t) \hat{\eta}(r, t) \rangle = \sum_q \left(|u_q(r, t)|^2 N_{BE}(\epsilon_q) + |v_q(r, t)|^2 (N_{BE}(\epsilon_q) + 1)\right)\] (4.6)

and

\[\tilde{m}(r, t) \equiv \langle \hat{\eta}(r, t) \hat{\eta}(r, t) \rangle = \sum_q u_q(r, t)v_q^*(r, t) (2N_{BE}(\epsilon_q) + 1)\] (4.7)

where \(N_{BE}(\epsilon_q)\) is the Bose distribution for the \(q\)th quasi-particle excitation given by (2.51)

\[N_{BE}(\epsilon_q) = \frac{1}{\exp(\beta\epsilon_q) - 1}.\] (4.8)

The condensate wavefunction \(\Phi(r, t)\) normalises according to

\[\int d\mathbf{r} |\Phi(r, t)|^2 = N - \tilde{N}\] (4.9)

where \(N\) is the total number of atoms, and \(\tilde{N}\) the total number of thermal atoms, and the quasi-particle amplitudes \(u_q(r, t)\) and \(v_q(r, t)\) according to (2.54), viz.

\[\int d\mathbf{r} \left(|u_q(r, t)|^2 - |v_q(r, t)|^2\right) = 1.\] (4.10)

The total number of thermal atoms \(\tilde{N}\) is obtained by integrating the thermal density \(\tilde{n}(r, t)\) over all space, thus

\[\tilde{N} = \int d\mathbf{r} \tilde{n}(r, t)\] (4.11)

In the frame rotating with angular frequency \(\Omega\) the single-particle Bose Hamiltonian is given by (2.25)

\[\hat{h}_\Omega(r) = -\frac{\hbar^2}{2m} \nabla^2 + i\hbar \Omega \cdot (r \times \nabla) + V_T(r).\] (4.12)

Likewise we can write the expression (2.26)

\[\hat{h}_v(r) = -\frac{\hbar^2}{2m} \nabla^2 + i\hbar \mathbf{v} \cdot \nabla + V_T(r)\] (4.13)

for the single-particle Bose Hamiltonian in the frame moving with translational velocity \(\mathbf{v}\).
4.2.2 The Continuity Equation for the Condensate Density

**In the Rotating Frame**  We find from the GGPE (4.3) for the rotating frame

\[
i\hbar \frac{\partial}{\partial t} \Phi(r, t) = \left( \hat{h}\Omega(r) - \mu + g \left( |\Phi(r, t)|^2 + 2\tilde{n}(r, t) \right) \right) \Phi(r, t) + g\tilde{m}(r, t)\Phi^*(r, t)
\]

and its complex conjugate, the continuity equation for the condensate density

\[
i\hbar \frac{\partial}{\partial t} |\Phi(r, t)|^2 = \frac{\hbar^2}{2m} \left( \Phi(r, t)\nabla^2\Phi^*(r, t) - \Phi^*(r, t)\nabla^2\Phi(r, t) \right) + i\hbar \Omega \cdot (r \times \nabla) |\Phi(r, t)|^2 + C(r, t)
\]

where we have defined the quantity

\[
C(r, t) \equiv g \left( \tilde{m}(r, t)\Phi^2(r, t) - \tilde{m}^*(r, t)\Phi^2(r, t) \right)
\]

related to the rate of change of the density of transfer of particles between the condensate and the thermal population. Defining the current density

\[
j(r, t) \equiv \frac{i\hbar}{2m} \left( \Phi(r, t)\nabla\Phi^*(r, t) - \Phi^*(r, t)\nabla\Phi(r, t) \right)
\]

yields the more usual form of the continuity equation for the condensate density

\[
\frac{\partial}{\partial t} |\Phi(r, t)|^2 + \nabla \cdot j(r, t) = \Omega \cdot (r \times \nabla) |\Phi(r, t)|^2 - \frac{i}{\hbar} C(r, t).
\]

**In the Translating Frame**  For the translating frame, we obtain the continuity equation for the condensate density

\[
i\hbar \frac{\partial}{\partial t} |\Phi(r, t)|^2 = \frac{\hbar^2}{2m} \left( \Phi(r, t)\nabla^2\Phi^*(r, t) - \Phi^*(r, t)\nabla^2\Phi(r, t) \right) + i\hbar v \cdot \nabla |\Phi(r, t)|^2 + C(r, t).
\]

In what follows, we shall make use of the time-independent version of equation (4.14) to calculate the precessional frequencies of vortices, and of equation (4.18) to calculate the translational velocity of topological defects in one dimension.

4.2.3 The time-independent HFB Equations

Stationary solutions for the GGPE and the BdGEs are found by substituting the form

\[
\Phi(r, t) = \Phi(r) \exp \left( -i\Delta \mu t/\hbar \right)
\]

\[(4.19)\]
for the condensate wave function into the time-dependent GGPE (4.3), and the forms
\[ u_q(r, t) = u_q(r) \exp(-i\epsilon_q t/\hbar) \]
\[ v_q(r, t) = v_q(r) \exp(-i\epsilon_q t/\hbar) \]
(4.20)
for the quasi-particle amplitudes into the time-dependent BdGEs (4.4), thereby obtaining the time-independent Generalised Gross Piteavskii equation (GGPE)
\[ (\Delta \mu + \mu) \Phi(r) = \left( \hat{h}(r) + g \left( |\Phi(r)|^2 + 2\tilde{n}(r) \right) \right) \Phi(r) + g\tilde{m}(r)\Phi^*(r) \]
(4.21)
and the time-independent Bogoliubov de Gennes Equations (BdGEs)
\[ \epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \begin{bmatrix} \hat{L}(r) & \mathcal{M}(r) \\ -\mathcal{M}^*(r) & -\hat{L}^*(r) \end{bmatrix} \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} \]
(4.22)
with
\[ \hat{L}(r) \equiv \hat{h}(r) - \mu + 2g \left( |\Phi(r)|^2 + \tilde{n}(r) \right) \]
\[ \mathcal{M}(r) \equiv g \left( \Phi^2(r) + \tilde{m}(r) \right) \]
(4.23)
\((\mu + \Delta \mu)\) and \(\epsilon_q\) are the respective eigenvalues corresponding to the GGPE and BdGEs, where \(\Delta \mu\) is the difference between the eigenvalue \((\mu + \Delta \mu)\) and the true chemical potential \(\mu\). \(\Delta \mu\) and \(\epsilon_q\) thus represent the condensate and quasi-particle energies relative to the system chemical potential \(\mu\). The populations of the quasi-particle states are given by the Bose distribution (4.8), and the ground state population is given likewise by the Bose distribution (A.30)
\[ N_c = N_{BE}(\Delta \mu) = \frac{1}{\exp(\beta \Delta \mu) - 1} \]
(4.24)
We find that [23, 24]
\[ \frac{\Delta \mu}{kT} = \ln \left( 1 + \frac{1}{N_c} \right) \approx \frac{1}{N_c} \]
(4.25)
for macroscopic occupation of the ground state (large condensate number \(N_c\)). So for \(kT \sim \mu\), i.e. our energy scale is of the order of the chemical potential, which holds for low temperature \(T\)
\[ \Delta \mu \sim \frac{\mu}{N_c}, \]
(4.26)
and we can neglect \(\Delta \mu\) in the low temperature regime. We note that \(\Delta \mu \to 0\) as \(N_c \to \infty\), i.e. \(\Delta \mu\) is zero in the thermodynamic limit. Thus the fugacity term
\[ Z = \exp \left( \frac{\Delta \mu}{k_B T} \right) \]
(4.27)
is very close to unity for low temperature \(T\), so we can ignore it when calculating the occupation numbers for the quasi-particle modes. The fugacity term referred to here is used in the calculation of the quasi-particle occupation numbers given by
\[ n_q = N_{BE}(\epsilon_q) = \frac{1}{Z^{-1} \exp(\beta \epsilon_q) - 1}. \]
(4.28)
and is due to the difference $\Delta \mu$ between the eigenvalue $(\mu + \Delta \mu)$ and the true chemical potential $\mu$. The usual definition for the fugacity in statistical mechanics is given by

$$Z = \exp \left( \frac{\mu}{k_B T} \right)$$

(4.29)

but here the the quasi-particle energies $\epsilon_q$ are already measured relative to the chemical potential $\mu$. Neglecting $\Delta \mu$, we obtain the time-independent GGPE

$$\mu \Phi(r) = \left( \hat{h}(r) + g (|\Phi(r)|^2 + 2\tilde{n}(r)) \right) \Phi(r) + g\tilde{m}(r)\Phi^*(r).$$

(4.30)

### 4.2.4 The HFB Hamiltonian

We obtain a quadratic approximation for the full Grand-Canonical Hamiltonian (4.1). This enables us to find an approximate diagonalisation of the Grand-Canonical Hamiltonian, and hence stationary solutions of the HFB equations. The eigenvalue of the GGPE would then represent the chemical potential of the system, and the energy eigenvalues of the BdGEs approximations of the collective excitations for the condensate. We see from linear response theory that the Bogoliubov approximation gives the collective excitations at $T = 0$ (see chapter 2). However for the full HFB, inconsistent treatment for the condensate and non-condensate due to the symmetry-breaking and the self-consistent mean-field approximation [11] leads to an unphysical gap in the quasi-particle energy spectrum. Later we shall see how this energy gap can be removed to reasonable approximation using perturbation theory.

Using the Bogoliubov decomposition $\hat{\psi}(r, t) = \Phi(r, t) + \hat{\eta}(r, t)$ and substituting into the Grand-Canonical Hamiltonian (4.1) and applying the mean field approximations (2.55) written in terms of the thermal and anomalous densities $\tilde{n}(r, t) \equiv \langle \hat{\eta}^\dagger(r, t)\hat{\eta}(r, t) \rangle$ and $\tilde{m}(r, t) \equiv \langle \hat{\eta}(r, t)\hat{\eta}(r, t) \rangle$ respectively, and the complex conjugate of the anomalous density $\tilde{m}^*(r, t) \equiv \langle \hat{\eta}^\dagger(r, t)\hat{\eta}^\dagger(r, t) \rangle$, we were able to approximate the Grand-Canonical Hamiltonian $\hat{H}^{(GC)}(t)$ by

$$\hat{H}^{(GC)}(t) \approx \hat{H}_{HFB}(t)$$

(4.31)

where we defined the HFB hamiltonian given by equations (2.57) and (2.58), breaking the HFB Hamiltonian into Hamiltonians of zeroth, first and second order in terms of the annihilation and creation fluctuation operators $\hat{\eta}$ and $\hat{\eta}^\dagger$, viz. (2.58). We now show that the time-independent HFB equations diagonalise the HFB Hamiltonian defined by equations (2.57) and (2.58):

Since $\int d\mathbf{r} \Phi^* \hat{h} \hat{\eta} = \int d\mathbf{r} \left( \hat{h}^\dagger \Phi^* \right) \hat{\eta}$ and $\int d\mathbf{r} \hat{\eta}^\dagger \hat{h} \hat{\eta} = \int d\mathbf{r} \left( \hat{h}^\dagger \hat{\eta}^\dagger \right) \hat{\eta}$ (see appendix B.1.2), we
can rewrite $\hat{H}_{\text{HFB}_1}$ and $\hat{H}_{\text{HFB}_2}$ in the form

$$\hat{H}_{\text{HFB}_1}(t) \equiv \int \! dr \left( \hat{\eta}^\dagger \left[ \left( \hat{\epsilon} - \mu + g \left| \Phi \right|^2 + 2\bar{n} \right) \hat{\Phi} + g\bar{n}\hat{\Phi}^* \right] + \text{h.c.} \right),$$  

(4.32)

$$\hat{H}_{\text{HFB}_2}(t) \equiv \int \! dr \left( \frac{1}{2} \hat{\eta}^\dagger \left[ \left( \hat{\epsilon} - \mu + 2g \left| \Phi \right|^2 + \bar{n} \right) \hat{\eta} + g \left( \hat{\Phi}^2 + \bar{m} \right) \hat{\eta}^\dagger \right] + \text{h.c.} \right).$$  

(4.33)

Then, substituting the Bogoliubov transformation (2.43) and the time-independent BdGEs (4.22) for the quasi-particle amplitudes into (4.32) and (4.33), we obtain from the orthogonality and symmetry relations (2.53) for the quasi-particle amplitudes, the following expression for the HFB Hamiltonian (see appendix A.1.3)

$$\hat{H}_{\text{HFB}} \equiv \int \! dr \left( \Phi^* \left( \hat{\epsilon} - \mu + \frac{g}{2} \left| \Phi \right|^2 \right) \Phi - g \left( \bar{\eta}^2 \hat{\Phi} + \frac{1}{2} \bar{\Phi}^2 \hat{\eta}^\dagger \right) + \sum_k \epsilon_k \left( \hat{n}_k - \int \! dr \left| \nu_k \right|^2 \right) \right)$$  

(4.34)

showing that the time-independent HFB equations (4.30) and (4.22) diagonalise the HFB Hamiltonian.

### 4.2.5 Conservation Laws

In any physical theory, it is essential that physical quantities such as total particle number, energy, angular and linear momentum, etc. are conserved. Here we demonstrate that this is the case for standard HFB, but that particle and both angular and linear momentum conservation are violated for Popov, and for the G1 and G2 gapless theories, rendering them unsuitable for time-dependent simulations.

**Particle Conservation**

**In the Rotating Frame** From the continuity equation for the condensate density (4.14) and the BdGEs (4.4) in the rotating frame, we find that the rate of change in the condensate and thermal populations are given respectively by (see appendix B.2.1)

$$\frac{dN_c(t)}{dt} = \frac{ig}{\hbar} \int \! dr \left( \bar{\eta}^* \Phi^2 \hat{\Phi} - \bar{\Phi}^2 \Phi^* \right)$$  

(4.35)

and

$$\frac{d\tilde{N}(t)}{dt} = \frac{ig}{\hbar} \int \! dr \left( \bar{\Phi}^* \Phi^2 \hat{\Phi} - \bar{\Phi}^2 \Phi^* \right)$$  

(4.36)

where the total number of condensate particles and the total number of thermal (non-condensate particles are given by $N_c(t) = \int \! dr \left| \Phi(r,t) \right|^2$ and $\tilde{N}(t) = \int \! d\bar{r} \bar{\eta}(r,t)$ respectively.
Therefore the rate of change of condensate particles is the negative of the rate of change of thermal particles, showing that particles are conserved for time-dependent HFB in the rotating frame, i.e.

\[
\frac{d}{dt} \left( N_c(t) + \tilde{N}(t) \right) = 0
\]  

(4.37)

**In the Translating Frame**

Particle conservation can also be proved in the case of the translating frame, where the rate of change for the condensate and thermal populations are given respectively by equations (4.35) and (4.36), and therefore the conservation of particles (4.37) holds.

It is evident from the above discussion that particles are conserved in general for HFB\(^1\).

**Violation of Particle Conservation for Popov, and for G1 and G2 Gapless Theories**

To show that particle conservation is violated for the Popov approximation, and for the gapless G1 and G2 theories, let us write the time-dependent GGPE and BdGEs for Popov, G1 and G2 as we did in equations (2.74)-(2.80). We obtain (see appendix B.2.1)

\[
\frac{dN_c}{dt} = ia \frac{g}{\hbar} \int d\mathbf{r} \left( \tilde{m} \Phi^* \Phi^2 - \tilde{m}^* \Phi^2 \right) + 2ib \frac{g}{\hbar} \int d\mathbf{r} \tilde{n} \left( \frac{\Phi^*}{\Phi} \Phi^* - \frac{\Phi}{\Phi} \Phi^* \right) 
\]  

(4.38)

and

\[
\frac{d\tilde{N}}{dt} = i \frac{g}{\hbar} \int d\mathbf{r} \left( \tilde{m}^* \Phi^2 - \tilde{m} \Phi^* \right) + 2ib \frac{g}{\hbar} \int d\mathbf{r} \tilde{n} \left( \frac{\Phi^*}{\Phi} \Phi^* - \frac{\Phi}{\Phi} \Phi^* \right) + 2ib \frac{g}{\hbar} \int d\mathbf{r} \tilde{n}^2 \left( \frac{\Phi^*}{\Phi} \Phi^* - \frac{\Phi}{\Phi} \Phi^* \right) 
\]  

(4.39)

Hence we find for Popov \((a = b = 0)\), for G1 \((a = 1, b = 0)\) and for G2 \((a = 1, b = 1)\) that (see appendix B.2.1)

\[
\frac{dN_c}{dt} \neq - \frac{d\tilde{N}}{dt}
\]  

(4.40)

so particle conservation is violated in all three cases. As a consequence of this, Popov, and the G1 and G2 gapless theories are unsuitable candidates for time-dependent simulations.

To explain this we note the scattering processes taken into account in mean-field theory as shown in figure 4.1. The terms responsible for the transfer of particles between the condensate and the non-condensate are \(\Phi^\dagger \tilde{\eta}^\dagger \tilde{\eta} \) which scatters particles from the condensate into the non-condensate, and \(\tilde{\eta}^\dagger \Phi^\dagger \tilde{\eta} \tilde{\eta} \) which scatters particles from the thermal population into the condensate. The respective ensemble-averaged terms are \(\Phi^2 \tilde{m}^*\) and \(\Phi^* \tilde{m} \), thus we see

\(^1\)One could also explain this by the fact that HFB is a phi-derivable, and hence a conserving theory [11, 89]. Therefore one would expect all physical conservation laws to be satisfied, including particle conservation.
that the anomalous density \( \tilde{m} \) plays a crucial role in the transfer of particles between the condensate and non-condensate. Hence the omission or modification of such terms leads to a violation of particle conservation. In the case of the Popov approximation, we have omitted the anomalous density entirely, therefore no transfer of particles to and from the condensate is possible, but the term \( \frac{d\tilde{N}}{dt} = i\hbar \int dr \left( \tilde{m}^* \Phi^4 - \tilde{m} \Phi^4 \right) \) implies that there is a transfer of particles to and from the thermal population, leading to a violation of particle conservation. This is a direct consequence of the inconsistency introduced by the neglect of the anomalous density. The same applies to the G1 and G2 theories. In the G1 and G2 theories, these terms have been modified, or extra terms introduced, leading to an imbalance in the transfer of particles between the condensate and the thermal population, therefore particle conservation is again violated.

**Energy Conservation**

We show that the HFB energy is a constant of the motion in the absence of an external time-dependent potential. Consider first a BEC in the presence of a time-varying potential \( V(\mathbf{r}, t) \), i.e. \( \hat{H}_{HFB} \rightarrow \hat{H}_{HFB} + V(\mathbf{r}, t) \). Then by the Heisenberg equation of motion

\[
\frac{i\hbar}{dt} \frac{d\hat{H}_{HFB}}{dt} = [\hat{H}_{HFB}, \hat{H}_{HFB}] + \int dr \left( \frac{i\hbar}{dt} \frac{\partial V}{\partial t} \right) \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t),
\]

and since any operator commutes with itself, and hence \([\hat{H}_{HFB}, \hat{H}_{HFB}] = 0\), we conclude that

\[
\frac{dE}{dt} = \left\langle \frac{d\hat{H}_{HFB}}{dt} \right\rangle = \left( \frac{\partial V}{\partial t} \right) \cdot \frac{d\hat{H}_{HFB}}{dt}.
\]

In the situation where the external (trapping) potential is time-independent, (i.e. \( \frac{\partial V}{\partial t} = 0 \)), \( \frac{dE}{dt} = \left\langle \frac{d\hat{H}_{HFB}}{dt} \right\rangle = 0 \), showing that energy is conserved. We show further that energy is also conserved for any perturbation scheme for HFB. The full Grand-Canonical
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Hamiltonian of equation (2.34) may be written

\[ \hat{H}^{(GC)}(t) \equiv \hat{H}_{HFB}(t) + \Delta \hat{H}_{13}(t) + \Delta \hat{H}_{24}(t) \]  
(4.43)

where \( \hat{H}_{HFB}(t) \) is the HFB Hamiltonian given by (2.57)

\[ \hat{H}_{HFB}(t) \equiv \hat{H}_{HFB_0}(t) + \hat{H}_{HFB_1}(t) + \hat{H}_{HFB_2}(t) \]  
(4.44)

where we have broken the HFB Hamiltonian into Hamiltonians of zeroth, first and second order in terms of the annihilation and creation fluctuation operators \( \hat{\eta} \) and \( \hat{\eta}^\dagger \) with \( \hat{H}_{HFB_0}(t) \) given by the first of equations (2.58), and \( \hat{H}_{HFB_1}(t) \) and \( \hat{H}_{HFB_2}(t) \) respectively by equations (4.32) and (4.33). In view of the approximate decomposition (2.55), the residual of the full Grand-Canonical Hamiltonian may be written \( \Delta \hat{H}(t) \equiv \Delta \hat{H}_{13}(t) + \Delta \hat{H}_{24}(t) \) where

\[ \Delta \hat{H}_{13}(t) = \Delta \hat{H}_1(t) + \Delta \hat{H}_3(t), \]
\[ \Delta \hat{H}_{24}(t) = \Delta \hat{H}_2(t) + \Delta \hat{H}_4(t) \]  
(4.45)

where the first, second, third and fourth order perturbation Hamiltonians in the thermal fluctuation operator \( \hat{\eta} \) are given by

\[ \Delta \hat{H}_1(t) = -g \int dr \left((2\Phi^* \hat{n} + \Phi m^*) \hat{\eta} + (2\Phi \hat{n} + \Phi^* m) \hat{\eta}^\dagger \right), \]
\[ \Delta \hat{H}_2(t) = -\frac{g}{2} \int dr \left(4\hat{n} \hat{\eta}^\dagger \hat{\eta} + \hat{m}^* \hat{\eta} \hat{\eta} + \hat{m} \hat{\eta}^\dagger \hat{\eta}^\dagger \right), \]
\[ \Delta \hat{H}_3(t) = g \int dr \left(\Phi^* \hat{\eta}^\dagger \hat{\eta} \hat{\eta} + \Phi \hat{\eta}^\dagger \hat{\eta}^\dagger \hat{\eta} \hat{\eta} \right), \]  
and
\[ \Delta \hat{H}_4(t) = \frac{g}{2} \int dr \hat{\eta} \hat{\eta}^\dagger \hat{\eta} \hat{\eta}, \]  
(4.46)

where we note that \( \Delta \hat{H}_3(t) \equiv \hat{H}_3^{(GC)} \), \( \Delta \hat{H}_4(t) \equiv \hat{H}_4^{(GC)} \). It can be shown that (see appendix B.2.2)

\[ \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{13}(t) \right] \right\rangle = \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{24}(t) \right] \right\rangle = 0 \]  
(4.47)

Hence for a time-independent external trapping potential,

\[ \left\langle i\hbar \frac{d\hat{H}_{HFB}(t)}{dt} \right\rangle = \left\langle \left[ \hat{H}_{HFB}(t), \hat{H}(t) \right] \right\rangle = \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{13}(t) \right] \right\rangle + \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{24}(t) \right] \right\rangle = 0 \]  
(4.48)

showing that energy is still conserved.

An alternative proof of the conservation of energy for HFB is shown at the end of appendix B.2.2, and reveals that energy conservation is violated in the cases of the Popov, G1 and G2 approximations.

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Conservation of Angular Momentum

One would expect the angular momentum of the BEC system to be conserved in the absence of any external potential, but that the introduction of an external potential may or may not affect the angular momentum of the system, depending on the symmetry properties of the external potential. We anticipate that the quantum expectation value of the angular momentum operator \( \hat{L} \) defined by \( \hat{L} \equiv i\hbar (\mathbf{r} \times \nabla) \) of the BEC be conserved in a spherically symmetric harmonic trap, and this will become evident shortly.

The quantum expectation value of the angular momentum is given by

\[
\langle \hat{L} \rangle = \left\langle \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r},t) \hat{L} \hat{\psi}(\mathbf{r},t) \right\rangle,
\]

and the rate of change of \( \langle \hat{L} \rangle \), the ensemble-averaged angular momentum of the BEC is given by

\[
\frac{d}{dt} \langle \hat{L} \rangle = \frac{d}{dt} \left\langle \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r},t) \hat{L} \hat{\psi}(\mathbf{r},t) \right\rangle.
\]

Substituting the time-dependent GGPE (4.3) and the time-dependent BdGEs (4.4) and their respective complex conjugates into (4.51) and applying the results in appendix B.1.2 for Bose field operators, we obtain (see appendix B.2.3)

\[
\frac{d}{dt} \langle \hat{L} \rangle = \frac{1}{i\hbar} \int d\mathbf{r} \left( |\Phi|^2 + \tilde{n} \right) \hat{L} V_T.
\]

The conservation of angular momentum therefore depends entirely on the trapping potential and/or any other externally applied potential, as one would expect. Angular momentum is conserved whenever \( \hat{L} V_T = 0 \). This is clearly the case whenever spherical symmetry exists, thus angular momentum is conserved in a spherically symmetric harmonic trap, i.e.

\[
\frac{d}{dt} \langle \hat{L} \rangle = 0.
\]

In an axially symmetric harmonic trap, \( \hat{L}_z V_T = 0 \), so the ensemble-averaged \( z \)-component (i.e. the component along the axis of symmetry) of angular momentum is conserved, i.e.

\[
\frac{d}{dt} \langle \hat{L}_z \rangle = 0.
\]
Clearly the angular momentum is always conserved in the absence of any trapping potential \((V_T = 0)\).

This holds for any linear differential operator \(D\), i.e. \(\frac{d}{dt}D = \int d\mathbf{r} \left( |\Phi|^2 + \tilde{n} \right) \hat{D}V_T\), therefore the same result applies to linear momentum.

### Violation of angular momentum conservation for Popov, G1 and G2

We show that conservation of the expectation value of the angular momentum \(\hat{L}\) of the BEC is violated for Popov, G1 and G2, whether a trapping potential is present or not.

From appendix B.2.3, we obtain the expression

\[
\frac{d \langle \hat{L} \rangle}{dt} = \int d\mathbf{r} \left( |\Phi|^2 + \tilde{n} \right) \hat{L}V_T + I_R \tag{4.55}
\]

where

\[
I_R = \frac{2g}{\hbar} \text{Re} \left\{ \frac{1}{i} \int d\mathbf{r} \left[ -(a - 1)\tilde{m}^* \Phi \hat{L} \Phi - 2b\tilde{m}^* \frac{\tilde{n} \Phi}{|\Phi|^2} \hat{L} \Phi - 2\tilde{m}^* \frac{(a |\Phi|^2 + b\tilde{n})}{\Phi^*} \langle \tilde{\eta}^\dagger \hat{L} \tilde{\eta} \rangle \right] \right\} \tag{4.56}
\]

For Popov \(a = b = 0\), for G1 \(a = 1, b = 0\), and for G2 \(a = b = 1\), \(I_R\) is given respectively by equations (B.68), (B.69) and (B.70) for Popov, G1 and G2. In general, \(I_R \neq 0\), so angular momentum conservation is violated in all three cases, regardless of the trapping potential, and this is illustrated in Appendix F, section F.1 in a time-dependent simulation (repeating the third time-dependent simulation carried out in section 7.5.2 of chapter 7) deploying the G1 approximation. In this simulation, the violation of number and angular momentum are clearly illustrated.

We see from the previous section that all physical conservation laws are observed for the full HFB formalism. This is not surprising since HFB is phi-derivable and hence a conserving theory \([11, 89]\).

#### 4.2.6 Calculation of the Angular Momentum in the Rotating Frame

The quantum expectation value of the angular momentum \(\hat{L}\) is given by

\[
\langle \hat{L} \rangle = \left\langle \int d\mathbf{r} \hat{\psi}^\dagger (\mathbf{r}, t) \hat{L} \hat{\psi} (\mathbf{r}, t) \right\rangle = \int d\mathbf{r} \left[ \Phi^* (\mathbf{r}, t) \hat{L} \Phi (\mathbf{r}, t) + \langle \tilde{\eta}^\dagger (\mathbf{r}, t) \hat{L} \tilde{\eta} (\mathbf{r}, t) \rangle \right] \tag{4.57}
\]
From the Bogoliubov transformation (2.43), and its Hermitian conjugate (2.44), and applying Wick’s theorem for ensemble averages of operator pairs $\hat{a}_k^\dagger \hat{a}_l$, we obtain the expression

$$\langle \hat{L} \rangle = i\hbar \int dr \left[ \Phi^* (\mathbf{r} \times \nabla) \Phi + \sum_q (n_q u_q^* (\mathbf{r} \times \nabla) u_q + (n_q + 1) v_q (\mathbf{r} \times \nabla) v_q^*) \right]$$

for $L$.

### 4.2.7 Calculation of the Precessional Frequency of Off-axis Vortices in Quasi-2D BECs

The precessional frequency of vortices may be predicted by using the time-independent HFB equations and the time-independent continuity equation for the condensate density to find the stationary solution for an off-axis vortex in the frame rotating at the precessional frequency of the vortex. The time-independent continuity equation for the condensate density is used to derive a suitable expression for the precessional frequency of off-axis vortices. We consider a stationary vortex system in the frame rotating at the precessional frequency of the off-axis vortex or vortices. This is solved self-consistently with the HFB equations in this rotating frame.

We derive a suitable expression for the rotational frequency from the time independent continuity equation for the condensate density (4.14) by writing the condensate wavefunction $\Phi(\mathbf{r}, t)$ in terms of its real and imaginary parts $R(\mathbf{r}, t)$ and $I(\mathbf{r}, t)$,

$$\Phi(\mathbf{r}, t) = R(\mathbf{r}, t) + iI(\mathbf{r}, t),$$

hence we find for a stationary solution ($\partial/\partial t |\Phi(\mathbf{r}, t)|^2 \equiv 0$)

$$\hbar \Omega \cdot (\mathbf{r} \times \nabla) |\Phi(\mathbf{r})|^2 = 2\frac{\hbar^2}{2m} \left( R(\mathbf{r}) \nabla^2 I(\mathbf{r}) - I(\mathbf{r}) \nabla^2 R(\mathbf{r}) \right) + iC(\mathbf{r})$$

where we have defined the quantity

$$C(\mathbf{r}) \equiv g \left( \tilde{m}(\mathbf{r}) \Phi^2(\mathbf{r}) - \tilde{m}^*(\mathbf{r}) \Phi^2(\mathbf{r}) \right).$$

It is convenient to represent the 2D system in polar coordinates (as we will be making use of the Laguerre polynomials for the basis functions). Writing $R \equiv R(\mathbf{r}, \theta)$, $I \equiv I(\mathbf{r}, \theta)$, we find that

$$\Omega r^2 A(r, \theta) = B(r, \theta)$$

where we have defined

$$A(r, \theta) \equiv \left( R \frac{\partial R}{\partial \theta} + I \frac{\partial I}{\partial \theta} \right)$$
and
\[ B(r, \theta) \equiv \frac{\hbar}{2m} \left[ r^2 \left( R \frac{\partial^2 I}{\partial r^2} - I \frac{\partial^2 R}{\partial r^2} \right) + r \left( R \frac{\partial I}{\partial r} - I \frac{\partial R}{\partial r} \right) + \left( R \frac{\partial^2 I}{\partial \theta^2} - I \frac{\partial^2 R}{\partial \theta^2} \right) \right] + \frac{r^2}{2\hbar} C(r, \theta) \] (4.63)

with
\[ C(r, \theta) \equiv g \left( \tilde{m} \Phi^* \Phi - \tilde{m}^* \Phi \Phi^* \right). \] (4.64)

Multiplying both sides by \( A(r, \theta) \), and integrating over all space gives us the expression
\[ \Omega = \frac{\int_0^{2\pi} \int_0^\infty A(r, \theta) B(r, \theta) rdr \theta}{\int_0^{2\pi} \int_0^\infty r^2 (A(r, \theta))^2 rdr \theta}. \] (4.65)

This result is important for two reasons:

1. It allows us to predict the precessional frequency for single off-axis vortices and for vortex arrays, allowing us to place the vortices in any desired position. For a single vortex one could choose a precessional frequency, solve the HFB equations self-consistently and then see where the vortex lies. However this does not provide us with a prediction of the precessional frequency of the vortices, and this procedure is not possible for vortex arrays. This provides us with a useful method for generating any desired vortex array, allowing us then to investigate the effect of symmetry-breaking of the trapping potential, the introduction of noise into the system by means of an external perturbing potential (i.e. \( \tilde{H}_{HFB} \rightarrow \tilde{H}_{HFB} + V(r, t) \)) where the externally applied potential \( V(r, t) \) consists of white noise, etc. using the time-dependent HFB equations to study the behaviour of the system.

2. This result demonstrates that the precession of the vortex is due to conservation of mass flow described by the continuity equation for the condensate density, and not by the LCLS energies as was originally asserted in [2, 3] - see chapter 7.

### 4.2.8 Calculation of the Translational Velocity of Topological Defects in 1D BECs in Toroidal Traps

We derive a similar expression for the translational velocity as follows. The time independent continuity equation for the condensate density in the translating frame is given by (4.18) and by writing \( \Phi(r, t) \) in terms of its real and imaginary parts (4.59) as before. We find for a stationary solution \((\partial/\partial t |\Phi(r, t)|^2 \equiv 0)\)
\[ \hbar v \nabla |\Phi(r)|^2 = 2\frac{\hbar^2}{2m} \left( R(r) \nabla^2 I(r) - I(r) \nabla^2 R(r) \right) + iC(r) \] (4.66)
For the 1D system we write \( R \equiv R(x), \ I \equiv I(x) \), obtaining

\[
v \left( R \frac{dR}{dx} + I \frac{\partial I}{\partial x} \right) = \frac{\hbar}{2m} \left( R \frac{d^2 I}{dx^2} - I \frac{d^2 R}{dx^2} \right) + \frac{ig}{2\hbar} \left( \bar{m} \Phi^* - \bar{m}^* \Phi \right). \tag{4.67}
\]

As for the 2D case, we multiply both sides by \( R \frac{dR}{dx} + I \frac{\partial I}{\partial x} \) and integrate over all space to obtain

\[
v = \frac{\int_{-\infty}^{\infty} A(x)B(x)dx}{\int_{-\infty}^{\infty} (A(x))^2 dx} \tag{4.68}
\]

where we have defined

\[
A(x) \equiv \left( R \frac{dR}{dx} + I \frac{\partial I}{\partial x} \right) \tag{4.69}
\]

and

\[
B(x) \equiv \frac{\hbar}{2m} \left( R \frac{d^2 I}{dx^2} - I \frac{d^2 R}{dx^2} \right) + \frac{i}{2\hbar} C(x) \tag{4.70}
\]

with

\[
C(x) \equiv g \left( \bar{m} \Phi^* - \bar{m}^* \Phi \right). \tag{4.71}
\]

Equations (4.65), (4.62) and (4.63) may be used to predict the precessional frequencies of off-axis vortices in the 2D system, and equations (4.68), (4.69) and (4.70) for the prediction of the translational velocities of topological defects in toroidal traps (1D system).

### 4.3 Orthogonal HFB

We wish to have a formalism in which the condensate population is orthogonal to the thermal population, in contrast with standard HFB. We shall see shortly that a zero-energy excitation exists in the orthogonal formalism, although this does not necessarily imply the existence of a Goldstone mode. This does not correct the quasi-particle energy spectrum, but at least now the lowest energy excitation is zero. Later we shall demonstrate that it is possible to correct the energy spectrum by calculating the quasi-particle energy shifts using second-order time-independent perturbation theory (section (4.3.8)), or alternatively using perturbation theory to remove the double counting of the anomalous density \( \bar{m} \) (latter part of section 4.3.8), thereby reproducing the Popov quasi-particle spectrum to a reasonable approximation, whilst still observing all conservation laws.

Let us split the Bose field operator \( \hat{\psi}(r, t) \) into a coherent part represented by the condensate field operator \( \hat{\Phi}(r, t) \), and an incoherent part represented by the fluctuation operator \( \hat{\eta}(r, t) \) and write (c.f. (2.160))

\[
\hat{\psi}(r, t) = \hat{\Phi}(r, t) + \hat{\eta}(r, t) \tag{4.72}
\]
where
\[ \hat{\Phi}(\mathbf{r}, t) \equiv \phi(\mathbf{r}, t)\hat{a}_c(t) \]  
(4.73)

with \( \hat{a}_c(t) \) and \( \hat{a}_c^\dagger(t) \) respectively the annihilation and creation operators for the condensate, where the condensate operator \( \hat{a}_c(t) \) is defined by (2.161), viz.
\[ \hat{a}_c(t) = \int d\mathbf{r} \phi^*(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t). \]  
(4.74)

and \( \phi(\mathbf{r}, t) \) some condensate wavefunction satisfying the normalisation condition (equation (2.162))
\[ \int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 = 1. \]  
(4.75)

The fluctuation operator \( \hat{\eta}(\mathbf{r}, t) \) is defined as in (2.163), viz.
\[ \hat{\eta}(\mathbf{r}, t) \equiv \hat{\psi}(\mathbf{r}, t) - \phi(\mathbf{r}, t) \int d\mathbf{r}'\phi^*(\mathbf{r}', t)\hat{\psi}(\mathbf{r}', t) \]  
(4.76)

and since
\[ \int d\mathbf{r} \phi^*(\mathbf{r}, t)\hat{\eta}(\mathbf{r}, t) = \int d\mathbf{r} \phi^*(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t) - \int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 \int d\mathbf{r} \phi^*(\mathbf{r}, t)\hat{\psi}(\mathbf{r}, t) = 0 \]
by the normalisation condition (4.75), we satisfy the orthogonality condition
\[ \int d\mathbf{r} \phi^*(\mathbf{r}, t)\hat{\eta}(\mathbf{r}, t) = 0 \]  
(4.77)

so the condensate and thermal populations are orthogonal, as required.

Since \( \hat{\psi}(\mathbf{r}, t) \) is a Bose field operator, it satisfies the Bose commutation relations
\[ \left[ \hat{\psi}(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t) \right] = \delta(\mathbf{r} - \mathbf{r}') \quad \left[ \hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t) \right] = 0 \quad \left[ \hat{\psi}^\dagger(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t) \right] = 0. \]  
(4.78)

The projection operator is defined by (2.164), viz.
\[ Q(\mathbf{r}, \mathbf{r}', t) \equiv \delta(\mathbf{r} - \mathbf{r}') - \phi(\mathbf{r}, t)\phi^*(\mathbf{r}', t). \]  
(4.79)

It can be shown from the commutation relations (4.78) and the definition (4.76) for the fluctuation operator \( \hat{\eta}(\mathbf{r}, t) \) that the following commutation relations hold (see appendix A.2.1):

1. The condensate operator \( \hat{a}_c(t) \) satisfies the Bose commutation relations
\[ \left[ \hat{a}_c(t), \hat{a}_c^\dagger(t) \right] = 1 \quad \text{and} \quad \left[ \hat{a}_c(t), \hat{a}_c(t) \right] = \left[ \hat{a}_c^\dagger(t), \hat{a}_c^\dagger(t) \right] = 0, \]  
(4.80)
2. the fluctuation operator \( \hat{\eta}(r, t) \) satisfies the quasi-Bosonic commutation relations

\[
[\hat{\eta}(r, t), \hat{\eta}^\dagger(r', t)] = Q(r, r', t) \quad \text{and} \quad [\hat{\eta}(r, t), \hat{\eta}(r', t)] = [\hat{\eta}^\dagger(r, t), \hat{\eta}^\dagger(r', t)] = 0,
\]

(4.81)

3. the condensate operator \( \hat{a}_c(t) \) and the fluctuation operator \( \hat{\eta}(r, t) \) commute, i.e.

\[
[\hat{a}_c(t), \hat{\eta}(r, t)] = [\hat{a}_c^\dagger(t), \hat{\eta}^\dagger(r, t)] = 0,
\]

(4.82)

4. and the condensate operator \( \hat{a}_c(t) \) and the Bose field operator \( \hat{\psi}(r, t) \) satisfy the commutation relations

\[
[\hat{a}_c(t), \hat{\psi}^\dagger(r, t)] = \phi^*(r, t) \quad \text{and} \quad [\hat{a}_c(t), \hat{\psi}(r, t)] = [\hat{a}_c^\dagger(t), \hat{\psi}^\dagger(r, t)] = 0.
\]

(4.83)

5. As a consequence the condensate and Bose field operators \( \hat{\Phi}(r, t) \) and \( \hat{\psi}(r, t) \) satisfy the commutation relations

\[
\left[\hat{\Phi}(r, t), \hat{\psi}^\dagger(r', t)\right] = \phi(r, t)\phi^*(r', t) \quad \text{and} \quad \left[\hat{\Phi}(r, t), \hat{\psi}(r', t)\right] = \left[\hat{\Phi}^\dagger(r, t), \hat{\psi}^\dagger(r', t)\right] = 0,
\]

(4.84)

6. and the fluctuation and Bose field operators \( \hat{\eta}(r, t) \) and \( \hat{\psi}(r, t) \) satisfy the commutation relations

\[
\left[\hat{\eta}(r, t), \hat{\psi}^\dagger(r', t)\right] = Q(r, r') \quad \text{and} \quad \left[\hat{\eta}(r, t), \hat{\psi}(r', t)\right] = \left[\hat{\eta}^\dagger(r, t), \hat{\psi}^\dagger(r', t)\right] = 0.
\]

(4.85)

Since the Bogoliubov transformation is canonical, the orthogonality and symmetry relations (2.53) still hold as before (see appendices A.1.2 and A.2.2). Using the commutation relations (4.78), (4.84) and (4.85) we have from the Heisenberg equations of motion for \( \hat{\Phi}(r, t), \hat{\eta}(r, t) \) and \( \hat{\psi}(r, t) \) for the full Grand-Canonical Hamiltonian (4.1) in the contact potential approximation, the respective dynamical equations

\[
i\hbar \frac{\partial \hat{\Phi}(r, t)}{\partial t} = \phi(r, t) \int dr' \phi^*(r', t) \left( \hat{h}(r') - \mu + g\hat{\psi}^\dagger(r', t)\hat{\psi}(r', t) \right) \hat{\psi}(r', t)
\]

(4.86)

\[
i\hbar \frac{\partial \hat{\eta}(r, t)}{\partial t} = \int dr' Q(r, r') \left( \hat{h}(r') - \mu + g\hat{\psi}^\dagger(r', t)\hat{\psi}(r', t) \right) \hat{\psi}(r', t)
\]

(4.87)

and

\[
i\hbar \frac{\partial \hat{\psi}(r, t)}{\partial t} = \left( \hat{h}(r) - \mu + g\hat{\psi}^\dagger(r, t)\hat{\psi}(r, t) \right) \hat{\psi}(r, t)
\]

(4.88)

Again we assume the existence of a weakly interacting quasi-particle basis, and apply the Bogoliubov transformation (2.43) and its Hermitian conjugate (2.44). We can apply the
commutation relations in equations (2.48), and the mean field approximations $\hat{a}_c\phi \rightarrow \Phi$, 
$\hat{\eta}^\dagger\hat{\eta} \rightarrow \langle \hat{\eta}^\dagger\hat{\eta} \rangle \equiv \bar{n}$, $\hat{\eta}\hat{\eta} \rightarrow \langle \hat{\eta}\hat{\eta} \rangle \equiv \bar{n}$, and $\hat{\eta}^\dagger\hat{\eta}^\dagger \rightarrow \langle \hat{\eta}^\dagger\hat{\eta}^\dagger \rangle \equiv \bar{m}^*$ to obtain the modified BdGEs

$$i\hbar \frac{\partial u_q(r,t)}{\partial t} = \int dr' \left( \hat{L}(r,r',t)u_q(r',t) + \mathcal{M}(r,r',t)v_q(r',t) \right)$$

(4.89)

and

$$-i\hbar \frac{\partial v_q(r,t)}{\partial t} = \int dr' \left( \hat{L}^*(r,r',t)v_q(r',t) + \mathcal{M}^*(r,r',t)u_q(r',t) \right)$$

(4.90)

where we have defined the operators $\hat{L}(r,r',t)$ and $\mathcal{M}(r,r',t)$

$$\hat{L}(r,r',t) \equiv Q(r,r',t)\hat{L}(r',t),$$

$$\mathcal{M}(r,r',t) \equiv Q(r,r',t)\mathcal{M}(r',t).$$

(4.91)

with $\hat{L}(r,t)$ and $\mathcal{M}(r,t)$ given by (4.5) as before. We have from equation (4.86)

$$\int dr\phi^*(r,t) \left( -i\hbar \frac{\partial \hat{\Phi}(r,t)}{\partial t} + (\hat{h}(r) - \mu + g\hat{\psi^\dagger}(r,t)\hat{\psi}(r,t)) \hat{\psi}(r,t) \right) = 0.$$  

(4.92)

Therefore we can write $i\hbar \frac{\partial \hat{\Phi}(r,t)}{\partial t}$ in the form

$$i\hbar \frac{\partial \hat{\Phi}(r,t)}{\partial t} = \left( \hat{h}(r) - \mu \right) \hat{\psi}(r,t) + g\hat{\psi^\dagger}(r,t)\hat{\psi}(r,t) + \hat{A}(r,t)$$

(4.93)

for some arbitrary operator $\hat{A}(r,t)$. Since the integrand is orthogonal to $\phi$, $\hat{A}(r,t)$ must therefore also be orthogonal to $\phi$, i.e.

$$\int dr\phi^*(r,t)\hat{A}(r,t) = 0.$$  

(4.94)

We choose $\hat{A}(r,t)$ such that all conservation laws are satisfied. We see from appendix B.3.2 and in what follows that choosing

$$\hat{A}(r,t) = -\frac{1}{\sqrt{N_c(t)}} \int dr' \left( \hat{\eta}^\dagger(r',t)\hat{L}(r',t) + \hat{\eta}(r',t)\mathcal{M}^*(r',t) \right) \phi(r',t)\hat{\eta}(r,t)$$

(4.95)

ensures that all conservation laws are satisfied. Taking expectation values thus gives us the modified GGPE

$$i\hbar \frac{\partial \Phi(r,t)}{\partial t} = \left( \hat{h}(r) - \mu + g \left( |\Phi(r,t)|^2 + 2\bar{n}(r,t) \right) \right) \Phi(r,t) + g\bar{n}(r,t)\Phi^*(r,t)$$

(4.96)

$$- \left\langle \int dr' \left( \hat{\eta}^\dagger(r',t)\hat{L}(r',t) + \hat{\eta}(r',t)\mathcal{M}^*(r',t) \right) \phi(r',t)\hat{\eta}(r,t) \right\rangle$$

since

$$\left\langle \hat{\psi}^\dagger(r,t)\hat{\psi}(r,t)\hat{\psi}(r,t) \right\rangle = (|\Phi(r,t)|^2 + 2\bar{n}(r,t)) \Phi(r,t) + \bar{m}(r,t)\Phi^*(r,t)$$
where $\Phi(r,t) \equiv \langle \hat{\Phi}(r,t) \rangle$, $\Phi^*(r,t) \equiv \langle \hat{\Phi}^+(r,t) \rangle$, $\tilde{n}(r,t) = \langle \hat{n}(r,t) \rangle$, $\tilde{m}(r,t) = \langle \hat{m}(r,t) \rangle$ as before. We defined in chapter 2, the normal and anomalous correlation densities (2.197)

$$
\tilde{n}(r',r,t) \equiv \langle \hat{n}(r',t)\hat{n}(r,t) \rangle = \sum_q \left[ u_q(r',t)u_q(r,t)N_{BE}(\epsilon_q) + v_q(r',t)v_q^*(r,t)(N_{BE}(\epsilon_q) + 1) \right]
$$

(4.97)

and (2.198)

$$
\tilde{m}(r',r,t) \equiv \langle \hat{m}(r',t)\hat{m}(r,t) \rangle = \sum_q \left[ v_q^*(r',t)u_q(r,t)N_{BE}(\epsilon_q) + u_q(r',t)v_q^*(r,t)(N_{BE}(\epsilon_q) + 1) \right].
$$

(4.98)

Clearly $\tilde{n}(r,t) \equiv \tilde{n}(r,r,t)$ and $\tilde{m}(r,t) \equiv \tilde{m}(r,r,t)$ represent the usual thermal and anomalous densities. Then defining the operator

$$
\hat{P}(r',r,t) \equiv \left( \tilde{n}(r',r,t)\hat{L}(r',t) + \tilde{m}(r',r,t)\hat{M}^*(r',t) \right) / \sqrt{N_c(t)}
$$

(4.99)

we obtain the modified GGPE

$$
i\hbar \frac{\partial \Phi(r,t)}{\partial t} = \left( \hat{h}(r) - \mu + g (|\Phi|^2 + 2\tilde{n}) \right) \Phi(r,t) + g\tilde{m}\Phi^*(r,t) - \int dr' \hat{P}(r',r,t)\phi(r',t)
$$

(4.100)

since

$$
\left\langle \int dr' \left( \hat{n}(r',t)\hat{L}(r',t) + \tilde{n}(r',t)\hat{M}^*(r',t) \right) \phi(r',t)\hat{n}(r,t) \right\rangle = \int dr' \hat{P}(r',r,t)\phi(r',t).
$$

(4.101)

We can derive the usual form (4.3) for the GGPE by neglecting the term $-\int dr' \hat{P}(r',r,t)\phi(r',t)$ or by taking the expectation value of the Heisenberg equation of motion for the Bose field operator $\hat{\psi}(r,t)$ (4.88)

$$
\frac{\partial \langle \hat{\psi}(r,t) \rangle}{\partial t} = \left\langle \left( \hat{h}(r) - \mu \right) \hat{\psi}(r,t) \right\rangle + g \langle \hat{\psi}^*(r,t)\hat{\psi}(r,t)\phi(r,t) \rangle.
$$

but then the conservation laws for linear and angular momentum are violated - see appendix B.3.2. Therefore, by the above and using the definition (4.91) for the operators $\hat{L}(r,r',t)$ and $\hat{M}(r,r',t)$, we have the modified (orthogonal) HFB equations consisting of the modified GGPE

$$
i\hbar \frac{\partial \Phi(r,t)}{\partial t} = \left( \hat{h}(r) - \mu + g (|\Phi|^2 + 2\tilde{n}) \right) \Phi(r,t) + g\tilde{m}\Phi^*(r,t) - \int dr' \hat{P}(r',r,t)\phi(r',t)
$$

(4.102)

and the modified (orthogonal) BdGEs

$$
i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(r,t) \\ v_q(r,t) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r,r',t) & \hat{M}(r,r',t) \\ -\hat{M}^*(r,r',t) & -\hat{L}^*(r,r',t) \end{bmatrix} \begin{bmatrix} u_q(r',t) \\ v_q(r',t) \end{bmatrix}.
$$

(4.103)
It is interesting to compare the modified GGPE with the GGPE used by Morgan et al. [60] in their linear response analysis on the generalised GPE subject to an external potential $P(r, t)$ given by (2.84), and here we compare the function $f(r, t)$ given by (2.85) with the projection part $\int dr' \hat{P}(r', r, t) \phi(r', t)$ of equation (4.102) above. Noting that

$$
\int dr' i \hbar \frac{\partial}{\partial t} \phi = - \int dr \phi \hat{h} \frac{\partial}{\partial r} \hat{n} = \int dr \phi \left[ \left( \hat{h}^* - \mu \right) \hat{\psi}^\dagger + g \hat{\psi} \hat{\psi}^\dagger \hat{\psi} \right]
$$

by the normalisation condition (4.75), substituting (4.102) into (4.101), and neglecting the projection part, we find that

$$
\int dr' \hat{P}(r', r, t) \phi(r', t) \approx g \int dr' \left( |\Phi(r', t)|^2 \phi(r', t) \hat{n}(r', r, t) + \Phi^*(r', t) \phi(r', t) \hat{\bar{m}}(r', r, t) \right) / \sqrt{N_c} + g \int dr' \left( -\hat{\bar{m}}(r', r, t) \phi^*(r', t) \hat{n}(r', r, t) + \hat{\bar{m}}^*(r', t) \phi(r', t) \hat{n}(r', r, t) \right) / \sqrt{N_c}
$$

Comparing this with (2.85), which we can rewrite as

$$
f(r, t) = g \int dr' \left( |\Phi(r', t)|^2 \phi(r', t) \hat{n}(r', r, t) + \Phi^*(r', t) \phi(r', t) \hat{\bar{m}}(r', r, t) \right) / \sqrt{N_c},
$$

we see the correspondence with equation (4.101) provided we neglect the second term in the right hand side of equation (4.104) and the remaining terms due to the projection operator $\hat{P}(r', r, t)$. We note therefore that whilst these forms of the GGPE are similar, the GGPE used by Morgan et al. [60] violates angular momentum conservation.

The corresponding time-independent orthogonal HFB equations are given by the modified time-independent GGPE

$$
\Delta \mu \Phi(r) = \left( \hat{h}(r) - \mu + g \left( |\Phi(r)|^2 + 2\hat{n}(r) \right) \right) \Phi(r) + g \hat{\bar{m}}(r) \Phi^*(r) - \int dr' \hat{P}(r', r) \phi(r')
$$

and the modified (orthogonal) BdGEs

$$
\epsilon_{\eta} \begin{bmatrix} u_{\eta}(r) \\ v_{\eta}(r) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r, r') & \hat{M}(r, r') \\ -\hat{M}^*(r, r') & -\hat{L}^*(r, r') \end{bmatrix} \begin{bmatrix} u_{\eta}(r') \\ v_{\eta}(r') \end{bmatrix}
$$

where the operators $\hat{L}, \hat{M}$ and $\hat{P}$ are now time-independent.

### 4.3.1 Existence of a Zero-Energy Excitation for Orthogonal HFB

To show the existence of a null subspace of zero energy eigenvalue modes for the orthogonal BdGEs spanned by the mode $(\phi, -\phi^*)$, let us write $u_0(r) = \alpha \phi(r), v_0(r) = -\beta \phi^*(r)$ for
some $\alpha, \beta \in \mathbb{C}$, where $\phi(r) = \Phi(r)/\sqrt{N_c}$, $\phi(r)$ is normalised to unity, i.e.

$$\int dr \left| \phi(r) \right|^2 = 1. \quad (4.108)$$

Then, substituting $u_0, v_0$ into the first of the modified time-independent BdGEs (4.107), we find that

$$\epsilon_0 \phi = \int dr' Q(r, r') \left[ \alpha \hat{L}(r', t) \phi(r') - \beta \hat{M}(r', t) \phi^*(r') \right]$$
$$= \alpha \hat{L}(r', t) \phi(r') - \beta \hat{M}(r', t) \phi^*(r')$$
$$- \phi(r) \int dr'^* \phi^*(r') \left[ \alpha \hat{L}(r', t) \phi(r') - \beta \hat{M}(r', t) \phi^*(r') \right].$$

Multiplying both sides by $\phi^*$, and integrating over all space, we find (in view of the orthonormality of $\phi$ and of the orthogonality condition (4.77)) that

$$\epsilon_0 = \phi(r) \int dr'^* \phi^*(r') \left[ \alpha \hat{L}(r', t) \phi(r') - \beta \hat{M}(r', t) \phi^*(r') \right]$$
$$- \phi(r) \int dr'^* \phi^*(r') \left[ \alpha \hat{L}(r', t) \phi(r') - \beta \hat{M}(r', t) \phi^*(r') \right]$$
$$= 0.$$

so there exists a zero-energy excitation. However, the existence of a zero energy eigenvalue does not imply that the Hugenholtz-Pines theorem [88] is satisfied or indeed that this corresponds to the Goldstone mode, nor is the remainder of the energy spectrum “corrected”, and is quite similar to the standard HFB spectrum in spite of the existence of a zero energy eigenvalue.

The existence of a Goldstone mode is important for the following reason. The Goldstone theorem for any non-relativistic field theory states that, for each spontaneously broken symmetry, there exists some quasi-particle with no energy gap. Here we break the symmetry when we select a preferred phase\(^2\) (as we do when making the classical field approximation, since the phase of the condensate field is arbitrary, and we select a preferred phase in specifying a c-number). Therefore by Goldstone’s theorem we would expect the existence of a quasi-particle with no energy gap corresponding to the existence of a Goldstone mode which is proportional to the condensate. The Hugenholtz-Pines theorem states more specifically that the quasi-particle spectrum associated with this symmetry-breaking process must be gapless. It is therefore essential that a Goldstone mode exists, and that the quasi-particle spectrum be gapless for the theory to be physical. Standard HFB does not satisfy this requirement, and is therefore an unphysical theory. Here by orthogonalising HFB, we now satisfy the requirement of a zero-energy excitation. However the Hugenholtz-Pines theorem is still not satisfied, nor does a Goldstone mode necessarily exist, and there

\(^2\)Symmetry is only broken when the operator becomes a c-number.
are still problems associated with the low-lying quasi-particle energy spectrum, and we shall demonstrate two methods by which this can be eliminated:

1. We use the second order perturbation results of Morgan (section 4.3.8) [23, 24] to obtain a quadratic approximation for the Grand-Canonical Hamiltonian (4.133) in terms of quasi-particle energy shifts that take into account the Beliaev and Landau processes. This should eliminate the energy gap in the lower-lying energies in the quasi-particle energy spectrum and reproduce a reasonable approximation for a quasi-particle energy spectrum that takes into account the Landau and Beliaev processes. These perturbative calculations do not affect number or angular momentum conservation. Since the time-independent formalism does not take into account the dynamics of the thermal cloud, we do not expect to reproduce accurately the Kohn mode frequency for the \( m = 1 \) mode in the time-independent calculations. The reason for this lies in the fact that the static thermal cloud presents an effective potential which reduces the \( m = 1 \) frequency by \( \sim 5\% \) for \( T \sim T_c/2 \) for the interaction strengths considered here, and hence does not produce the Kohn frequency (i.e. Kohn’s theorem is not rigorously observed). However, as we shall see in Chapter 5, the time-dependent HFB theory does obey Kohn’s Theorem rigorously.

2. We can use first-order and second-order perturbation theory to remove the effect of double counting of \( \tilde{m} \) (see latter part of section 4.3.8), rather than simply ignoring \( \tilde{m} \) to achieve an essentially gapless quasi-particle energy spectrum. This yields the Popov quasi-particle energy spectrum to a reasonable approximation without violating number and angular momentum conservation.

### 4.3.2 The Continuity Equation for the Condensate Density

**In the Rotating Frame** We find from the modified GGPE (4.102) for the rotating frame

\[
i\hbar \frac{\partial}{\partial t} \Phi(r, t) = \left( \hbar \Omega(r) - \mu + g (|\Phi|^2 + 2\tilde{n}) \right) + g\tilde{m}\Phi^*(r, t) - \int d r' \hat{P}(r', r, t) \phi(r', t) \tag{4.109}
\]

and its complex conjugate, the continuity equation for the condensate density

\[
i\hbar \frac{\partial}{\partial t} |\Phi(r, t)|^2 = \frac{\hbar^2}{2m} \left( \Phi(r, t) \nabla^2 \Phi^*(r, t) - \Phi^*(r, t) \nabla^2 \Phi(r, t) \right) + i\hbar \Omega \cdot (r \times \nabla) |\Phi(r, t)|^2 + C(r, t) \tag{4.110}
\]
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where we now define the quantity \( C(\mathbf{r}, t) \) by

\[
C(\mathbf{r}, t) \equiv g \left( \hat{m}(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) - \hat{m}^*(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) \right) + G^*(\mathbf{r}, t) - G(\mathbf{r}, t)
\]  

(4.111)

with

\[
G(\mathbf{r}, t) \equiv \Phi^*(\mathbf{r}, t) \int d\mathbf{r}' \hat{P}(\mathbf{r}', t) \phi(\mathbf{r}', t).
\]  

(4.112)

The corresponding time-independent continuity equation for the condensate density is given by

\[
\frac{\hbar^2}{2m} \left( \Phi(\mathbf{r}) \nabla^2 \Phi^*(\mathbf{r}) - \Phi^*(\mathbf{r}) \nabla^2 \Phi(\mathbf{r}) \right) + i\hbar \Omega \cdot (\mathbf{r} \times \nabla) |\Phi(\mathbf{r})|^2 + C(\mathbf{r}) = 0.
\]  

(4.113)

In the Translating Frame  For the translating frame, we obtain the continuity equation for the condensate density

\[
i\hbar \frac{\partial}{\partial t} |\Phi(\mathbf{r}, t)|^2 = \frac{\hbar^2}{2m} \left( \Phi(\mathbf{r}, t) \nabla^2 \Phi^*(\mathbf{r}, t) - \Phi^*(\mathbf{r}, t) \nabla^2 \Phi(\mathbf{r}, t) \right) + i\hbar \mathbf{v} \cdot \nabla |\Phi(\mathbf{r}, t)|^2 + C(\mathbf{r}, t)
\]  

(4.114)

with corresponding time-independent continuity equation for the condensate density

\[
\frac{\hbar^2}{2m} \left( \Phi(\mathbf{r}) \nabla^2 \Phi^*(\mathbf{r}) - \Phi^*(\mathbf{r}) \nabla^2 \Phi(\mathbf{r}) \right) + i\hbar \mathbf{v} \cdot \nabla |\Phi(\mathbf{r})|^2 + C(\mathbf{r}) = 0.
\]  

(4.115)

4.3.3 Particle Conservation for Orthogonal HFB

Having established an orthogonal formalism, it is now important to show that the conservation laws are still observed, as is the case with standard HFB. We begin with particle conservation.

Since

\[
\int d\mathbf{r} d\mathbf{r}' \Phi^*(\mathbf{r}, t) \hat{P}(\mathbf{r}', t) \phi(\mathbf{r}', t) = \int d\mathbf{r} d\mathbf{r}' \Phi(\mathbf{r}, t) \hat{P}^*(\mathbf{r}', t) \phi^*(\mathbf{r}', t) = 0
\]

by the orthogonality relation (4.77), we obtain from the continuity equation for the condensate density (4.109) for the modified GGPE in the rotating frame (or alternatively, equation (4.114) in the translating frame) the expression

\[
\frac{dN_c(t)}{dt} = \frac{g}{\hbar} \int d\mathbf{r} \left( \hat{m}(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) - \hat{m}^*(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) \right)
\]  

(4.116)

for the rate of change for the condensate population, as before. We find when substituting the modified BdGEs (4.103) into the expression

\[
\frac{d\tilde{N}(t)}{dt} = i\hbar \int d\mathbf{r} \left\langle \left( i\hbar \frac{\partial \hat{n}^\dagger}{\partial t} \right) \hat{n} + \hat{n}^\dagger \left( i\hbar \frac{\partial \hat{n}}{\partial t} \right) \right\rangle
\]

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for the total number of thermal particles, and applying the orthogonality relation (4.77) (see appendix B.3.1) that
\[
\frac{d\tilde{N}(t)}{dt} = i\frac{g}{\hbar} \int d\mathbf{r} \left( \tilde{m}^*(\mathbf{r}, t)\Phi^2(\mathbf{r}, t) - \tilde{m}(\mathbf{r}, t)\Phi^*\Phi(\mathbf{r}, t) \right)
\] (4.117)
and therefore that (4.37) holds, i.e.
\[
\frac{d}{dt} \left( N_c(t) + \tilde{N}(t) \right) = 0
\] (4.118)
showing that particles are conserved for time-dependent orthogonal HFB.

### 4.3.4 Conservation of Energy for Orthogonal HFB

Energy conservation is not affected in any way by this orthogonalisation, since we use the same HFB Hamiltonian. As previously,
\[
\frac{dE}{dt} = \left\langle \frac{d\hat{H}_{\text{HFB}}}{dt} \right\rangle = 0
\] (4.119)
for a time-independent external (trapping) potential, and energy is conserved as in the case for standard HFB.

### 4.3.5 Conservation of Angular Momentum for Orthogonal HFB

We verify in appendix B.3.2 that our choice of (4.99) for the operator \( \hat{P}(\mathbf{r}', \mathbf{r}, t) \) does indeed allow for the conservation of angular and linear momentum. We start with angular momentum, and show that the expectation value of the angular momentum \( \hat{L} \) of the BEC is conserved in a spherically symmetric harmonic trap.

The rate of change of \( \hat{L} \) is given by (4.50)
\[
\frac{d}{dt} \left\langle \hat{L} \right\rangle = \frac{d}{dt} \left\langle \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}, t) \hat{L} \hat{\psi}(\mathbf{r}, t) \right\rangle
\] (4.120)
where \( \hat{L} = i\hbar (\mathbf{r} \times \nabla) \) is the angular momentum operator, and since \( \hat{\psi}(\mathbf{r}, t) = \hat{\Phi}(\mathbf{r}, t) + \hat{\eta}(\mathbf{r}, t) \) by (4.72), we find that
\[
\frac{d}{dt} \left\langle \hat{L} \right\rangle = \frac{1}{i\hbar} \left\langle \int d\mathbf{r} \left[ i\hbar \frac{\partial}{\partial t} \hat{\Phi}^\dagger \hat{L} \hat{\Phi} + \hat{\Phi}^\dagger \hat{L} \left( i\hbar \frac{\partial}{\partial t} \hat{\Phi} \right) + i\hbar \frac{\partial}{\partial t} \hat{\eta}^\dagger \hat{L} \hat{\eta} + \hat{\eta}^\dagger \hat{L} \left( i\hbar \frac{\partial}{\partial t} \hat{\eta} \right) \right] \right\rangle
\] (4.121)
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Hence substituting the modified GGPE (4.102) and the orthogonal BdGEs (4.103) and their respective complex conjugates into the above equation, and applying the orthogonality condition (4.77) $\int dr \phi^*(r, t) \hat{\eta}(r, t) = 0$ and its Hermitian conjugate $\int dr \phi(r, t) \hat{\eta}^d(r, t) = 0$, and from the definition (4.73) for the condensate operator $\hat{\Phi}(r, t) \equiv \phi(r, t) \hat{a}_c(t)$, we obtain (see appendix B.3.2)

$$\frac{d}{dt} \langle \hat{L} \rangle = \int dr \left( |\Phi|^2 + \hat{n} \right) \hat{L} V_T$$  \hspace{1cm} (4.122)

as before. Again angular momentum is conserved in a spherically symmetric harmonic trap ($\hat{L} V_T = 0$), i.e.

$$\frac{d}{dt} \langle \hat{L} \rangle = 0$$  \hspace{1cm} (4.123)

and in an axially symmetric harmonic trap, where $\hat{L}_z V_T = 0$,

$$\frac{d}{dt} \langle \hat{L}_z \rangle = 0$$  \hspace{1cm} (4.124)

so the $z$-component of the angular momentum is conserved. Clearly the angular momentum is always conserved in the absence of any trapping potential ($V_T = 0$), as was the case for standard HFB. The conservation of linear momentum also holds, since the result (4.122) is true for any operator having the form of a linear differential operator $\hat{D}$.

4.3.6 Calculation of the Precessional Frequency of Off-axis Vortices in Quasi-2D BECs in the Orthogonal Formalism

The calculation here is similar to standard HFB, but with the introduction of an additional term due to the operator $\hat{P}$ - see continuity equation for the condensate density (4.110) and equations (4.111) and (4.112) for orthogonal HFB. From the time-independent continuity equation for the condensate density (4.113) for the orthogonal formalism, we find for the 2D system in polar coordinates upon multiplying both sides by $\left( R \frac{\partial R}{\partial r} + I \frac{\partial I}{\partial \theta} \right)$, and integrating over all space (as we did in section 4.2.7), we obtain (4.65) as before, but where $C(r, \theta)$ is now defined by

$$C(r, \theta) \equiv g \left( \hat{m}(r, \theta) \Phi^2(r, \theta) - \hat{m}^*(r, \theta) \Phi^2(r, \theta) \right) + G^*(r, \theta) - G(r, \theta),$$  \hspace{1cm} (4.125)

with

$$G(r, \theta) \equiv \Phi^*(r, \theta) \int_0^{2\pi} \int_0^\infty r' dr' d\theta' \hat{P}(r', \theta', r, \theta) \phi(r', \theta')$$  \hspace{1cm} (4.126)

and the projection operator $\hat{P}(r', \theta', r, \theta)$ in polar coordinates given by

$$\hat{P}(r', \theta', r, \theta) = \left( \hat{n}(r', \theta', r, \theta) \hat{L}(r', \theta') + \hat{m}(r', \theta', r, \theta) \hat{M}^*(r', \theta') \right) / \sqrt{N_c}.$$  \hspace{1cm} (4.127)
4.3.7 Calculation of the Translational Velocity of Topological Defects in 1D BECs in Toroidal Traps in the Orthogonal Formalism

From the time-independent continuity equation for the condensate density (4.115) for the orthogonal formalism in the frame moving with velocity $v$, we obtain (4.68) for the 1D system as before, but where $C(x)$ is now defined by

$$C(x) \equiv g \left( \tilde{m}(x)\Phi^*(x) - \tilde{m}^*(x)\Phi(x) \right) + G^*(x) - G(x)$$

(4.128)

where

$$G(x) \equiv \Phi^*(x) \int_{-\infty}^{\infty} dx' \hat{P}(x', x) \phi(x')$$

(4.129)

with the projector operator $\hat{P}(x, x')$ in the cartesian variable $x$ given by

$$\hat{P}(x', x) = \left( \tilde{n}(x', x)\hat{L}(x') + \tilde{m}(x', x)M^*(x') \right) / \sqrt{N_c}.$$  

(4.130)

4.3.8 Perturbation Theory for Orthogonal HFB

Perturbation Theory for Orthogonal HFB as per [23, 24]

As alluded to earlier, we can use the second order perturbation results of Morgan (chapter 2, section 2.6.2) [23, 24] to obtain a quadratic approximation for the Grand-Canonical Hamiltonian (4.133). This should effectively remove the energy gap in the low-lying quasi-particle energy spectrum, and provide a reasonable approximation to the quasi-particle energy spectrum, taking into account the Landau and Beliaev processes.

If we rewrite the expressions $\Delta \hat{H}_1$, $\hat{H}_3$, and $\hat{H}_4$ in Morgan’s treatment [23,24] in the position representation in the contact potential approximation, we find that

$$\Delta \hat{H}_1 = -g \int dr \left[ (2\Phi^*\tilde{n} + \Phi\tilde{m}^*) \hat{\eta} + (2\Phi\tilde{n} + \Phi^*\tilde{m}) \hat{\eta}^\dagger \right],$$

$$\hat{H}_3 = g \int dr \left( \Phi^*\tilde{\eta}^\dagger\tilde{\eta} + \Phi\tilde{\eta}^\dagger\tilde{\eta}^\dagger \right),$$

and

$$\hat{H}_4 = \frac{g}{2} \int dr \tilde{\eta}^\dagger\tilde{\eta}^\dagger\tilde{\eta} \tilde{\eta}.$$

We see a direct correspondence with the perturbation Hamiltonians $\Delta \hat{H}_1$, $\Delta \hat{H}_3$, and $\Delta \hat{H}_4$ in equations (4.45) and (4.46). In Morgan’s treatment [23, 24] $\Delta \hat{H}_2$ is given by

$$\Delta \hat{H}_2 \approx 2g \int dr \left( |\Phi(2)|^2 - |\Phi(0)|^2 \right) \tilde{\eta}^\dagger\tilde{\eta} + \frac{g}{2} \int dr \left( \Phi(2)^2 - \Phi(0)^2 \right) \tilde{\eta}^\dagger\tilde{\eta}^\dagger + \text{h.c.}$$
where \( \Phi^{(2)}(\mathbf{r}) \) is the solution to the GGPE, and \( \Phi^{(0)}(\mathbf{r}) \) the solution to the GPE. Now from the normalisation conditions \( \int d\mathbf{r} \left( |\Phi^{(2)}(\mathbf{r})|^2 + \tilde{n} \right) = \int d\mathbf{r} |\Phi^{(0)}(\mathbf{r})|^2 = 1 \) for the GGPE and GPE condensate wave-functions, we deduce that \( \Phi^{(2)} - \Phi^{(0)} \sim -\tilde{\eta} \) so \( |\Phi^{(2)}|^2 - |\Phi^{(0)}|^2 \sim -\tilde{n} \), and \( \Phi^{(2)^2} - \Phi^{(0)^2} \sim -\tilde{m} \), hence \( \Delta \hat{H}_2 \sim -\frac{2}{\hbar} \int d\mathbf{r} \left( 4\tilde{\eta}^\dagger \tilde{\eta} + \tilde{m}^\dagger \tilde{m} + \tilde{m} \tilde{m}^\dagger \right) \), i.e. is of the same order as \( \Delta \hat{H}_2 \) in (4.46). Therefore we can neglect \( \Delta \hat{H}_{24} = \Delta \hat{H}_2 + \Delta \hat{H}_4 \) thus allowing us to associate the perturbation Hamiltonian in S. A. Morgan’s treatment [23, 24] with the perturbation Hamiltonian \( \Delta \hat{H}_{13} + \Delta \hat{H}_{24} \) in equation (4.43). This enables us to apply the second order perturbation theory results of S. A. Morgan [23, 24] in order to calculate the shifts in the quasi-particle energies \( \Delta E_3(q) \) given by the expression (2.151), where

\[
\Delta E_3(q) = \sum_{i,j \neq 0} \left[ -\frac{|A_{qij}^{P3}|^2}{2(\epsilon_q + \epsilon_i + \epsilon_j)} + \frac{|B_{qij} + B_{qji}|^2}{2(\epsilon_q - \epsilon_i - \epsilon_j)} + \frac{|B_{ijq} + B_{qij}|^2}{(\epsilon_q - \epsilon_i + \epsilon_j)} \right] (4.131)
\]
as in [23, 24] is the energy shift due to a single quasi-particle mode \( q \) due to \( \Delta \hat{H}_{13} \). Neglecting the energy shift due to the quartic term \( \Delta \hat{H}_{24} \), we can write

\[
\Delta \hat{H}_{13} + \Delta \hat{H}_{24} \approx \sum_k \Delta \epsilon_k \hat{n}_k \quad (4.132)
\]

where we have identified \( \Delta \epsilon_q \equiv \Delta E_3(q) \) with \( \Delta E_3(q) \) given by the expression (4.131) since there are \( n_k \) quasi-particles in state \( k \) with associated number operator \( \hat{n}_k \). Since \( \left\langle i\hbar \frac{d}{dt} \left( \Delta \hat{H}_{13}(t) + \Delta \hat{H}_{24}(t) \right) \right\rangle = 0 \) by equation (4.47), these energy shifts can be considered to be time-independent in the mean-field approximation, allowing us to use these energy shifts in the time-dependent HFB. Incorporating (4.132) into the Grand-Canonical Hamiltonian given by equations (4.43) and (4.44), we now have the quadratic approximation in terms of the HFB Hamiltonian \( \hat{H}_{HFB}(t) \) and the quasi-particle energy shifts \( \Delta \epsilon_k \) given by equation (4.131)\(^3\)

\[
\hat{H}^{(GC)}(t) \approx \hat{H}_{HFB}(t) + \sum_k \Delta \epsilon_k \hat{n}_k. \quad (4.133)
\]

The quantities \( A_{ijk}^{P3}, A_{ijk} \) and \( B_{ijk} \) in equation (4.131) are defined according to [23, 24], where \( A_{ijk}^{P3} \equiv A_{ijk} + A_{ikj} + A_{jik} + A_{kij} + A_{kji} \), with \( A_{ijk} \) and \( B_{ijk} \) given by (2.147) and (2.148). In the position representation, using the contact potential approximation, \( A_{ijk} \) and \( B_{ijk} \) are given by

\[
A_{ijk} = \int d\mathbf{r} \left( \Phi^* v_i u_j u_k + \Phi u_i v_j v_k \right) \quad (4.134)
\]

\(^3\)Since we have a quadratic approximation for the Grand-Canonical Hamiltonian which also takes into account cubic and quartic terms in \( \tilde{\eta} \) and \( \tilde{\eta}^\dagger \), and therefore the Landau and Beliaev processes, we are now justified in applying Wick’s Theorem for thermal averages (see for example [87]).
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and

\[ B_{ijk} = \int d\mathbf{r} (\Phi^* (u_i^* u_j u_k + v_i^* v_j u_k + v_i^* u_j v_k) + \Phi (u_i^* u_j v_k + u_i^* v_j u_k + v_i^* v_j v_k)). \] (4.135)

Using this result and noting that \( \langle \left[ \sum_k \Delta \epsilon_k \hat{n}_k, \hat{\eta}_q \right] \rangle = \Delta \epsilon_q u_q \), we now have the modified GGPE (4.102) (which remains unaffected)

\[ i\hbar \frac{\partial \Phi(\mathbf{r}, t)}{\partial t} = \left( \hat{h}(\mathbf{r}) - \mu + g (|\Phi|^2 + 2\tilde{n}) \right) \Phi(\mathbf{r}, t) + g\tilde{n}\Phi^*(\mathbf{r}, t) - \int d\mathbf{r}' \hat{P}(\mathbf{r}', \mathbf{r}) \phi(\mathbf{r}', t) \] (4.136)
as before, and the modified time-dependent orthogonal BdGEs (c.f. (4.103))

\[ i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(\mathbf{r}, t) \\ v_q(\mathbf{r}, t) \end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix} \hat{L}(\mathbf{r}, \mathbf{r}', t, \Delta \epsilon_q) & \mathcal{M}(\mathbf{r}, \mathbf{r}', t) \\ -\mathcal{M}^*(\mathbf{r}, \mathbf{r}', t) & -\hat{L}^*(\mathbf{r}, \mathbf{r}', t, -\Delta \epsilon_q) \end{bmatrix} \begin{bmatrix} u_q(\mathbf{r}', t) \\ v_q(\mathbf{r}', t) \end{bmatrix} \] (4.137)

with

\[ \hat{L}(\mathbf{r}, \mathbf{r}', t, \Delta \epsilon_q) \equiv \hat{L}(\mathbf{r}, \mathbf{r}', t) + \Delta \epsilon_q \delta(\mathbf{r} - \mathbf{r}') \] (4.138)

where the operators \( \hat{P}(\mathbf{r}', \mathbf{r}, t) \), \( \hat{L}(\mathbf{r}, \mathbf{r}', t) \) and \( \mathcal{M}(\mathbf{r}, \mathbf{r}', t) \) are defined as before (equations (4.99) and (4.91)). We calculate the energy shifts \( \Delta \epsilon_q \) using equations (4.131), (4.134) and (4.135).

The motivation behind this is to find a quadratic approximation for the Grand-Canonical Hamiltonian that also takes into account the Landau and Beliaev processes that are neglected in standard HFB. This should remove the inconsistencies created in neglecting the third order term on the Grand-Canonical Hamiltonian for reasons similar to those presented by Morgan [23, 24], and hence lead to a gapless orthogonal HFB formalism. This new quadratic approximation for the Grand-Canonical Hamiltonian should provide motivation for the time-dependent orthogonal HFB formalism. A zero-energy excitation exists regardless of whether or not the energy shifts are included (see section 4.3.1). Neglecting these energy shifts will simply cause the thermal and anomalous densities to be slightly under-estimated and hence will not affect the results on the precession of vortices (chapter 7) qualitatively. In this thesis we ignore these energy shifts, but we don’t expect this to affect the results here in any significant way.

The corresponding time-independent HFB equations may now be written

\[ \Delta \mu \Phi(\mathbf{r}) = \left( \hat{h}(\mathbf{r}) - \mu + g (|\Phi(\mathbf{r})|^2 + 2\tilde{n}(\mathbf{r})) \right) \Phi(\mathbf{r}) + g\tilde{n}(\mathbf{r})\Phi^*(\mathbf{r}) - \int d\mathbf{r}' \hat{P}(\mathbf{r}', \mathbf{r}) \phi(\mathbf{r}') \] (4.139)

and

\[ \epsilon_q \begin{bmatrix} u_q(\mathbf{r}) \\ v_q(\mathbf{r}) \end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix} \hat{L}(\mathbf{r}, \mathbf{r}', \Delta \epsilon_q) & \mathcal{M}(\mathbf{r}, \mathbf{r}') \\ -\mathcal{M}^*(\mathbf{r}, \mathbf{r}') & -\hat{L}^*(\mathbf{r}, \mathbf{r}', -\Delta \epsilon_q) \end{bmatrix} \begin{bmatrix} u_q(\mathbf{r}') \\ v_q(\mathbf{r}') \end{bmatrix} \] (4.140)
which differs from the equations derived by Morgan [23, 24] in that the energy shifts appear only as on-diagonal terms. In order to simplify the numerical implementation, we re-write equation (4.140) as

$$
\varepsilon_q^{(U)} \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \int \! dr' \begin{bmatrix} \hat{L}(r, r') & \mathcal{M}(r, r') \\ -\mathcal{M}^*(r, r') & -\hat{L}^*(r, r') \end{bmatrix} \begin{bmatrix} u_q(r') \\ v_q(r') \end{bmatrix} \tag{4.141}
$$

where the eigenvalues of the orthogonal time-independent BdGEs \( \varepsilon_q^{(U)} = \varepsilon_q - \Delta \varepsilon_q \) are the unperturbed quasi-particle excitation energy values. Solving the time-independent HFB equations (4.139) and (4.141) self-consistently together with the quasi-particle energy shifts \( \Delta \varepsilon_q \equiv \Delta E_3(q) \) given by equation (4.131) yields the unperturbed quasi-particle energy spectrum and the energy shifts, and hence the perturbed (gapless) energy spectrum [23, 24]

$$
\varepsilon_q = \varepsilon_q^{(U)} + \Delta \varepsilon_q. \tag{4.142}
$$

Alternatively, one could solve the GGPE (4.139), and a set of modified BdGEs along the lines of (2.156), (2.157), and (2.158) as in [23, 24], i.e. of the form (see equation (D.36))

$$
\varepsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \int \! dr' \begin{bmatrix} \hat{L}^{(P)}(r, r', \epsilon_q) & \mathcal{M}^{(P)}(r, r', \epsilon_q) \\ -\mathcal{M}^{(P)*}(r, r', -\epsilon_q) & -\hat{L}^{(P)*}(r, r', -\epsilon_q) \end{bmatrix} \begin{bmatrix} u_q(r') \\ v_q(r') \end{bmatrix} \tag{4.143}
$$

where we have defined the perturbed operators \( \hat{L}^{(P)}(r, r', \epsilon_q) \) and \( \mathcal{M}^{(P)}(r, r', \epsilon_q) \) (see (D.37)) for quasi-particle \( q \) having energy \( \epsilon_q \) by

$$
\hat{L}^{(P)}(r, r', \epsilon_q) \equiv \hat{L}(r, r') + \Delta \hat{L}(r, r', \epsilon_q)
$$

$$
\mathcal{M}^{(P)}(r, r', \epsilon_q) \equiv \mathcal{M}(r, r') + \Delta \mathcal{M}(r, r', \epsilon_q) \tag{4.144}
$$

where \( \Delta \hat{L}(r, r', \epsilon_q) \) and \( \Delta \mathcal{M}(r, r', \epsilon_q) \) are as defined in equations (D.38), but this is numerically more difficult, and the form (4.137) for the modified orthogonal time-dependent BdGEs lends credence to time-dependent HFB. Apart from the presence of the operator \( Q(r, r') \) in the equations (D.38), the equations (4.143) and (4.144) are the same as those derived by Morgan [23, 24] written in the position representation, i.e. the \( \Delta \hat{L}'(r, r', \epsilon_q) \) and

---

4The modified BdGEs (4.143) are obtained by noting that the quasi-particle energy shifts \( \Delta \varepsilon_q \) can be written in the quadratic form in \( u_q \) and \( v_q \) given by (D.33), and can thus be incorporated into the unperturbed time-independent BdGEs (4.103) as indicated in Appendix D.1.2. This is then consistent with the form (4.143) where \( \Delta \hat{L}(r, r', \epsilon_q) \) and \( \Delta \mathcal{M}(r, r', \epsilon_q) \) are defined by equations (D.38). It should be noted that although the forms (4.140) and (4.143) both use the same quasi-particle energy shifts (4.131), they are not exactly equivalent. The form (4.140) for the modified BdGEs is preferable since it is consistent with the time-dependent modified BdGEs (4.137) which, together with the time-dependent GGPEs (4.136), satisfy the important conservation laws already discussed.
the $\Delta M'(r, r', \epsilon_q)$ given respectively by (D.34) and (D.35) are exactly equivalent to equations (2.153) and (2.154) written in the position representation. The effect of the shifted energies on the time-dependent HFB simulations is relatively small, so the effect on the calculations and simulations in this thesis of ignoring the shifts in the energies is sufficiently small that the results remain qualitatively correct in the limit of mean-field theory.

Use of Perturbation Theory to eliminate Double-counting of $\tilde{m}$

We follow the arguments of Proukakis [15–17] concerning the double-counting of $\tilde{m}$ (also discussed in Chapter 2), but avoid the difficulties of the Popov approximation concerning the violation of number and angular momentum conservation by removing the effect of $\tilde{m}$ perturbatively rather than by simply just ignoring it. This effectively removes the energy gap associated with the double-counting of $\tilde{m}$ and retrieves the Popov spectrum to a good approximation, without violating any conservation laws. As argued in the previous section, neglecting these energy shifts does not affect the results on the precession of vortices in chapter 7 qualitatively, and we don’t expect the results on vortex precession to be affected in any significant way. The respective shifts in the chemical potential and quasi-particle energies derived in Appendix D.2 are given by

$$\Delta \mu = \Delta \mu^{(1)} + \Delta \mu^{(2)} \quad (4.145)$$

and

$$\Delta \epsilon_q = \Delta \epsilon_q^{(1)} + \Delta \epsilon_q^{(2)}. \quad (4.146)$$

Here

$$\Delta \mu^{(1)} = -\frac{g}{2} \int d\mathbf{r} \left( \phi_0^2(\mathbf{r}) \tilde{m}^*(\mathbf{r}) + \phi_0^2(\mathbf{r}) \tilde{m}(\mathbf{r}) \right) \quad (4.147)$$

and

$$\Delta \epsilon_q^{(1)} = -\frac{g}{k} \int d\mathbf{r} \left( u_q^{(0)*} (\mathbf{r}) u_q^{(0)} (\mathbf{r}) \tilde{m}(\mathbf{r}) + u_q^{(0)} (\mathbf{r}) v_q^{(0)*} (\mathbf{r}) \tilde{m}^*(\mathbf{r}) \right) \quad (4.148)$$

for the first-order shifts, and

$$\Delta \mu^{(2)} = g^2 \sum_{n \neq 0} \left[ \int d\mathbf{r} (\phi_n \phi_n^* \tilde{m}^* + \phi_n^* \phi_n^* \tilde{m}) \int d\mathbf{r} (\phi_0 \phi_0^* \tilde{m}^* + \phi_0^* \phi_0^* \tilde{m}) \right] \quad (4.149)$$

and

$$\Delta \epsilon_q^{(2)} = g^2 \sum_{n \neq q} \left[ \int d\mathbf{r} \left( u_n^{(0)*} v_q^{(0)} \tilde{m} + v_n^{(0)*} u_q^{(0)} \tilde{m}^* \right) \int d\mathbf{r} \left( u_q^{(0)*} v_n^{(0)} \tilde{m} + v_q^{(0)*} u_n^{(0)} \tilde{m}^* \right) \right] \quad (4.150)$$
for the second-order shifts. We apply these results by solving the GGPE (4.106), with the shift in the chemical potential (4.145), the BdGEs (4.107) with the shifted chemical potential, viz.

\[
\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r, r', -\Delta \mu) & \hat{M}(r, r') \\ -\hat{M}^*(r, r') & -\hat{L}^*(r, r', -\Delta \mu) \end{bmatrix} \begin{bmatrix} u_q(r') \\ v_q(r') \end{bmatrix}
\]

with

\[
\hat{L}(r, r', \Delta \mu) \equiv \hat{L}(r, r') + \Delta \mu \delta(r - r')
\]

(c.f. (4.138) and the energy shifts (4.146) self-consistently. This calculation does not significantly increase the computational effort already required in solving the orthogonal HFB equations, and reproduces the Popov quasi-particle energy spectrum to reasonable accuracy (the errors are relatively small, typically \(\sim 1 - 2\%\)) and is therefore useful in calculating the thermal densities more accurately.

### Applicability of Perturbation Theory for Orthogonal HFB

In both perturbation techniques the quasi-particle energy spectrum is reproduced to reasonable accuracy (< 5% in extreme cases). Since only the low-lying quasi-particle energies are affected significantly by these calculations, the thermal densities may be calculated to quite good accuracy in both cases\(^5\). In the parameter regime considered here, the differences due to the energy shifts are relatively small (typically 2 – 3%), and hence do not significantly affect the results in this thesis. Calculations not presented here indicate that the differences in the predicted transition temperature in the non-vortex case are also quite small, with the transition temperature being slightly over-estimated in the unperturbed case. They are in reasonable agreement with the Popov prediction which predicts a slightly lower transition temperature. Further studies (also not presented here) indicate that the Popov prediction for the vortex case under-estimates the transition temperature, whereas the predictions for the unperturbed and perturbed orthogonal HFB calculations for the vortex case remain in reasonable agreement, being slightly over-estimated in the unperturbed case. The predicted transition temperatures for the vortex case tend to be lower than for the non-vortex case, but the Popov calculations produce predicted transition temperatures that are unreasonably low in the vortex case. We conclude that the perturbation

---

\(^5\)Some perturbation calculations using the perturbation scheme defined by equations (4.145)-(4.152) have been performed for a BEC in the absence of any vortices for a mode cut-off of 209, and are presented in appendix F.2.
calculations do not have a significant effect on either the thermal density or the predicted transition temperature $T_c$.

In this way we justify the omission of perturbative calculations in the work done in this thesis. The perturbative calculations could be included, but this would imply extra computational effort which, in the light of the above discussion, is unnecessary for the purposes of this thesis.
Chapter 5

Numerical Methods

5.1 Introduction

In this chapter we present methods used to solve the time-independent and the time-dependent orthogonal HFB equations\(^1\) in the regimes of axial symmetry and of tight axial confinement. We also present methods of computing gradients accurately required for the calculation of precessional frequencies of vortices using the continuity equation for the condensate density. This is achieved by analytic differentiation and pre-calculation of the first and second order partial derivatives of the Laguerre basis functions with respect to the radial and azimuthal coordinates \(r\) and \(\theta\) respectively. Before discussing the various numerical techniques used, let us represent the orthogonal HFB equations in dimensionless form.

---

\(^1\)The numerical algorithms presented here relate to the orthogonal HFB formalism. It is easy, however, to adapt these methods to standard HFB. In the numerical work done here, all time-independent calculations were done in the orthogonal formalism, whereas the time-dependent simulations were done mostly using the standard HFB formalism to reduce the computational effort, and because this is also numerically more robust. However, some of these calculations have been repeated using the orthogonal formalism, and the differences found to be insignificant.
5.2 Computational Units for BEC in Axially Symmetric Harmonic Trap

5.2.1 Computational Units for 3D system

We consider an axially symmetric harmonic trap, and define the length scale

\[ r_0 = \sqrt{\frac{\hbar}{m\omega_r}} \]  

(5.1)

and the time scale

\[ t_0 = \frac{2}{\omega_r} \]  

(5.2)

so that the dimensionless forms (denoted by primes) now become

\[
\begin{align*}
    r &= r_0 r' \\
    t &= t_0 t'.
\end{align*}
\]  

(5.3)

It is also useful to use dimensionless forms for the condensate wave function, for the quasiparticle amplitudes and for the condensate and non-condensate densities

\[
\begin{align*}
    \Phi(r, t) &= \sqrt{N/r_0^3} \Phi'(r, t) \\
    u_q(r, t) &= \sqrt{N/r_0^3} u_q'(r, t) \\
    v_q(r, t) &= \sqrt{N/r_0^3} v_q'(r, t)
\end{align*}
\]  

(5.4)

Consequently

\[
\begin{align*}
    n_c(r, t) &= (N/r_0^3) n_c'(r, t) \\
    \tilde{n}(r, t) &= (N/r_0^3) \tilde{n}'(r, t) \\
    \tilde{m}(r, t) &= (N/r_0^3) \tilde{m}'(r, t)
\end{align*}
\]  

(5.5)

The energies are now given in harmonic oscillator units

\[ E_0 = \frac{\hbar \omega_r}{2} \]  

(5.6)

Thus we have, for example \( \mu = E_0 \mu' \). Substituting (5.1) - (5.6) into the modified GGPE (4.102), the BdGEs (4.103), and the expressions (4.5) and (4.99) for the operators \( \hat{\mathcal{L}}(r, t) \), \( \mathcal{M}(r, t) \), and \( \hat{P}(r', r, t) \), and dropping the primes denoting dimensionless units for notational convenience, we obtain the dimensionless forms

\[
\begin{align*}
    i \frac{\partial \Phi(r, t)}{\partial t} &= \left( \hat{h} - \mu + C_{3D} \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi(r, t) + C_{3D} \tilde{m} \Phi(r, t') - \int d\mathbf{r}' \hat{P}(r', r, t) \phi(r', t)
\end{align*}
\]  

(5.7)
for the modified GGPE, and
\[
i \frac{\partial}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r, r', t) & \mathcal{M}(r, r', t) \\ -\mathcal{M}^*(r, r', t) & -\hat{L}^*(r, r', t) \end{bmatrix} \begin{bmatrix} u_q(r', t) \\ v_q(r', t) \end{bmatrix}
\] (5.8)
for the modified BdGEs, where
\[
\hat{P}(r', r, t) \equiv \tilde{n}(r', r, t) \hat{L}(r', t) + \tilde{m}(r', r, t) \mathcal{M}^*(r', t)
\] (5.9)
and
\[
\hat{L}(r, r', t) \equiv Q(r, r', t) \hat{L}(r', t)
\]
\[
\mathcal{M}(r, r', t) \equiv Q(r, r', t) \mathcal{M}(r', t).
\] (5.10)
Here
\[
\hat{L}(r, t) \equiv \hat{h}(r) - \mu + 2 C_{3D} (|\Phi(r, t)|^2 + \tilde{n}(r, t))
\]
\[
\mathcal{M}(r, t) \equiv C_{3D} (\Phi^2(r, t) + \tilde{m}(r, t))
\] (5.11)
and
\[
\hat{h}(r) = -\nabla^2 - \mu + r^2 + \lambda^2 z^2
\] (5.12)
where, in cylindrical coordinates
\[
\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}
\] (5.13)
with the trap aspect ratio \(\lambda\) defined by
\[
\lambda \equiv \frac{\omega_z}{\omega_r},
\] (5.14)
and where the nonlinearity constant \(C_{3D}\) is given by
\[
C_{3D} = 8\pi a_s N.
\] (5.15)
Here \(N\) is the number of atoms, \(a_s\) is the s-wave scattering length, and \(r_0\) is the length scale as defined above. In the frame rotating with angular frequency \(\Omega\), the single Boson Hamiltonian is given by
\[
\hat{h}_\Omega(r) = -\nabla^2 + i \Omega \cdot (r \times \nabla) + r^2 + \lambda^2 z^2
\] (5.16)
and by
\[
\hat{h}_v(r) = -\nabla^2 + i v \cdot \nabla + r^2 + \lambda^2 z^2
\] (5.17)
in the frame moving with constant velocity \(v\). The dimensionless condensate wavefunction \(\Phi(r, t)\) and the quasiparticle amplitudes \(u_q(r, t)\) and \(v_q(r, t)\) now normalise according to
\[
\int d\mathbf{r} |\Phi(r, t)|^2 = 1 - \frac{\bar{N}}{N}
\] (5.18)
where $N$ is the total number of atoms, and $\tilde{N} = N \int d\mathbf{r} \tilde{n}(\mathbf{r}, t)$ is the total number of thermal atoms for the condensate wavefunction, and

$$\int d\mathbf{r} \left( |u_q(\mathbf{r}, t)|^2 - |v_q(\mathbf{r}, t)|^2 \right) = \frac{1}{N}$$

(5.19)

for the quasiparticle amplitudes.

The corresponding time-independent orthogonal HFB equations are given by the dimensionless modified time-independent GGPE

$$\Delta \mu \Phi(\mathbf{r}) = \left( \hat{h} - \mu + C_{3D} \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi(\mathbf{r}) + C_{3D} \tilde{m} \Phi^*(\mathbf{r}) - \int d\mathbf{r}' \hat{P}(\mathbf{r}, \mathbf{r}') \phi(\mathbf{r}')$$

(5.20)

and the dimensionless BdGEs

$$\epsilon_q \begin{bmatrix} u_q(\mathbf{r}) \\ v_q(\mathbf{r}) \end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix} \hat{\mathcal{L}}(\mathbf{r}, \mathbf{r}') & \mathcal{M}(\mathbf{r}, \mathbf{r}') \\ -\mathcal{M}^*(\mathbf{r}, \mathbf{r}') & -\hat{\mathcal{L}}^*(\mathbf{r}, \mathbf{r}') \end{bmatrix} \begin{bmatrix} u_q(\mathbf{r}') \\ v_q(\mathbf{r}') \end{bmatrix}$$

(5.21)

where the operators $\hat{P}$, $\hat{\mathcal{L}}$ and $\mathcal{M}$ are now time-independent.

### 5.2.2 Computational Units for Quasi-2D System

In the numerical calculations in chapters 6 and 7, we use the same length and time scales (5.1) and (5.2) as in section 5.2.1, and the same dimensionless forms (5.7) for the GGPE and (5.8) for the BdGEs. The condensate wavefunction and quasiparticle amplitudes are in units of $\sqrt{N/r_0^3}$ as in (5.4), and the energies are given in harmonic oscillator units $\hbar \omega_r/2$ as in (5.6).

We consider an axially symmetric harmonic trap where the axial trapping frequency $\omega_z$ is much larger than the radial trapping frequency $\omega_r$, i.e. $\omega_z \gg \omega_r$. Thus the trap aspect ratio $\lambda = \omega_z/\omega_r \gg 1$. In this regime the energy of the first excited state in the axial direction is sufficiently high compared to the radial energy levels that, provided the temperature $T$ is sufficiently low, i.e. $k_B T \ll \hbar \omega_z$, and we can, to a good approximation, ignore all excited states in the axial direction. The quasi-two-dimensional approximation holds provided the axial harmonic transition energy $\hbar \omega_z$ is much greater than the temperature $T$ and the mean-field energy of the BEC [95]. The axial harmonic energy corresponds to a temperature $T_{\Delta z} = \hbar \omega_z/k_B$, and the mean field energy to an effective temperature of $T_{MF} = C_{2D} n_0/k_B'$, where $k_B$ is Boltzmann’s constant, and $k_B' = 2k_B/(\hbar \omega_r)$. In all simulations in this thesis, $T_{\Delta z} = 19.2\text{nK}$, $T_{MF} \approx 0.84\text{nK}$, and $T \lesssim 12.5\text{nK}$ for the BEC cooling simulations, and $T \lesssim 7.5\text{nK}$ for the vortex calculations, so this approximation is justified. We can thus
write the condensate wavefunction in the form
\[ \Phi(r, t) = \phi_m(r, \theta, t) Z_0(z) \] (5.22)
where \( Z_0(z) \) is the lowest axial particle state (see appendix C.1.2)
\[ Z_0(z) = N_0 e^{-\lambda z^2/2} \] (5.23)
where
\[ N_0 = \left( \frac{\lambda}{\pi} \right)^{1/4} \] (5.24)
similarly we can write the quasiparticle amplitudes as
\[
\begin{align*}
  u_q(r, t) &= u_q(r, \theta, t) Z_0(z) \\
  v_q(r, t) &= v_q(r, \theta, t) Z_0(z).
\end{align*}
\] (5.25)
Then
\[
\begin{align*}
  n_c(r, t) &= n_c(r, \theta, t) |Z_0(z)|^2 \\
  \tilde{n}(r, t) &= \tilde{n}(r, \theta, t) |Z_0(z)|^2 \\
  \tilde{m}(r, t) &= \tilde{m}(r, \theta, t) |Z_0(z)|^2.
\end{align*}
\] (5.26)
We substitute these forms into the three-dimensional, dimensionless forms for the GGPE (5.7) and the BdGEs (5.8), and integrate over all \( z \), making use of the orthogonality properties of \( Z_k(z) \) and the eigenvalue equation for the 1D harmonic oscillator (C.10)
\[ \left(-\frac{d^2}{dz^2} + \lambda z^2\right) Z_k(z) = \lambda (2k + 1) Z_k(z) \] (5.27)
(see appendix C.1.2). Thus we obtain the orthogonal HFB equations for the 2D system comprising the 2D GGPE
\[ i \frac{\partial \Phi}{\partial t} = \left( \hat{h} - \mu + C_{2D} (|\Phi|^2 + 2\tilde{n}) \right) \Phi + C_{2D} \tilde{m} \Phi^* - \int_0^{2\pi} \int_0^{\infty} r' dr' d\theta' \hat{P}(r', \theta', r, \theta, t) \phi(r', \theta', t) \] (5.28)
and the 2D Bogoliubov de Gennes Equations (BdGEs)
\[
\begin{align*}
  i \frac{\partial}{\partial t} \begin{bmatrix} u_q(r, \theta, t) \\ v_q(r, \theta, t) \end{bmatrix} &= \begin{bmatrix} \hat{L}(r, \theta, r', \theta', t) & \hat{M}(r, \theta, r', \theta', t) \\ -\hat{M}^*(r, \theta, r', \theta', t) & \hat{L}^*(r, \theta, r', \theta', t) \end{bmatrix} \begin{bmatrix} u_q(r', \theta', t) \\ v_q(r', \theta', t) \end{bmatrix}
\end{align*}
\] (5.29)
where
\[
\begin{align*}
  \hat{L}(r, \theta, r', \theta', t) &\equiv Q(r, \theta, r', \theta', t) \hat{L}(r', \theta', t) \\
  \hat{M}(r, \theta, r', \theta', t) &\equiv Q(r, \theta, r', \theta', t) \hat{M}(r', \theta', t)
\end{align*}
\] (5.30)
with
\[ \hat{L}(r, \theta, t) \equiv \hat{h}(r, \theta) - \mu + 2C_{2D} \left( |\Phi(r, \theta, t)|^2 + \bar{n}(r, \theta, t) \right) \]
\[ \mathcal{M}(r, \theta, t) \equiv C_{2D} \left( \Phi^2(r, \theta, t) + \bar{m}(r, \theta, t) \right) \]
and the operators \( Q(r, \theta, r', \theta') \) and \( \hat{P}(r', \theta', r, \theta, t) \) given respectively by
\[ Q(r, \theta, r', \theta') = \frac{1}{r'} \delta(r - r') \delta(\theta - \theta') - \phi(r, \theta) \phi^*(r', \theta') \] (5.31)
and
\[ \hat{P}(r', \theta', r, \theta, t) \equiv \left( \bar{n}(r', \theta', r, \theta, t) \hat{L}(r', \theta', t) + \bar{m}(r', \theta', r, \theta, t) \mathcal{M}^*(r', \theta', t) \right) \sqrt{N_c(t)}. \] (5.32)

Here
\[ \hat{h}(r, \theta) = - \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right) + r^2 \] (5.33)
and the shift \( \lambda \) has been incorporated into the chemical potential \( \mu \), i.e. \( \mu - \lambda \to \mu \). The nonlinearity constant \( C_{2D} \) is given in terms of the three-dimensional non-linearity constant \( C_{3D} \) (5.15) by integrating over all \( z \), i.e.
\[ C_{2D} = \int_{-\infty}^{\infty} dz \left| Z_0(z) \right|^4 C_{3D}. \] We find that
\[ C_{2D} = 8\pi \left( \frac{\lambda}{2\pi} \right)^{1/2} \frac{a_s}{r_0} N. \] (5.34)
where \( N \) is the number of atoms, \( a_s \) is the s-wave scattering length, and \( r_0 \) is the length scale as defined above. In the frame rotating with angular frequency \( \Omega \), the single Boson Hamiltonian \( \hat{h}_\Omega(r, \theta) \) is given by
\[ \hat{h}_\Omega(r, \theta) = - \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right) + i\Omega \frac{\partial}{\partial \theta} + r^2. \] (5.35)
The time independent 2D orthogonal HFB equations in the rotating frame are then given by the 2D time-independent GGPE
\[ \mu \Phi = \left( \hat{h}_\Omega + C_{2D} \left( |\Phi|^2 + 2\bar{n} \right) \right) \Phi + C_{2D} \bar{m} \Phi^* - \int_0^{2\pi} \int_0^\infty r' dr' d\theta' \hat{P}(r', \theta', r, \theta) \phi(r', \theta') \] (5.36)
and the 2D time-independent Bogoliubov de Gennes Equations (BdGEs)
\[ \epsilon_q \begin{bmatrix} u_q(r, \theta) \\ v_q(r, \theta) \end{bmatrix} = \int_0^{2\pi} \int_0^\infty r' dr' d\theta' \begin{bmatrix} \hat{L}(r, \theta, r', \theta') & \mathcal{M}(r, \theta, r', \theta') \\ -\mathcal{M}^*(r, \theta, r', \theta') & -\hat{L}^*(r, \theta, r', \theta') \end{bmatrix} \begin{bmatrix} u_q(r', \theta') \\ v_q(r', \theta') \end{bmatrix}. \] (5.37)
5.3 Numerical Solutions of the Time-independent HFB Equations

The regime of interest here is the axially symmetric harmonically confined quasi-2D BEC (tight axial confinement). We shall consider the cases of an axially symmetric BEC in the absence of vortices, or with a single on-axis vortex, and the more general non-axially-symmetric BEC (which may have several off-axis vortices). In the former case, the azimuthal coordinate $\theta$ may be integrated out producing a set of radial HFB equations, and in the second case we have a two dimensional set of equations in the radial coordinate $r$ and the azimuthal coordinate $\theta$. In both cases the axial confinement is considered to be sufficiently strong such that all excitations in the axial direction may be ignored, and the axial coordinate $z$ integrated out to produce a one or a two-dimensional problem with a suitably modified non-linearity parameter - see section 5.2.2.

In all cases we expand the condensate wave-function $\Phi(r)$ and the quasi-particle amplitudes $u_q(r)$ and $v_q(r)$ in terms of the single-particle basis functions $\xi_k(r)$. These single-particle basis functions are solutions of the (single-particle) time-independent Schrödinger equation with respective energy eigenvalues $\mu_{k}^{(SP)}$, viz.

$$\mu_{k}^{(SP)}\xi_k(r) = \hat{h}(r)\xi_k(r) \quad (5.38)$$

Thus we may write the condensate wave function $\Phi(r)$ as

$$\Phi(r) = \sum_k a_{0k}\xi_k(r) \quad (5.39)$$

and the quasiparticle amplitudes $u_q(r)$ and $v_q(r)$ as

$$u_q(r) = \sum_k c_{qk}\xi_k(r) \quad (5.40)$$

and

$$v_q(r) = \sum_k d_{qk}\xi_k(r) \quad (5.41)$$

respectively. In this way we obtain matrix (eigenvalue) equations for the coefficients $a_{jk}$ for the condensate wave-function $\Phi(r)$ (we use the lowest energy eigenvector for condensate wave-function, and hence the coefficients $a_{0k}$), and for the coefficients $c_{qk}$ and $d_{qk}$ for the quasi-particle amplitudes $u_q(r)$ and $v_q(r)$ written in terms of the respective matrix elements. We obtain the following matrix equations. For the coefficients for the condensate wavefunction (GGPE) we obtain (see appendix C.2.1)

$$\mu a = (A + B) a \quad (5.42)$$
and for the quasiparticle amplitudes (BdGEs) the matrix equation

\[ \begin{bmatrix} \epsilon_q & c_q \\ \begin{bmatrix} \mathbf{L}^{(u)}_q \\ -\mathbf{M}^{(v)}_q \\ -\mathbf{L}^{(v)}_q \end{bmatrix} & \end{bmatrix} \begin{bmatrix} \mathbf{d}_q \\ \begin{bmatrix} \mathbf{c}_q \\ \mathbf{d}_q \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \mathbf{L}^{(u)}_q \\ \begin{bmatrix} \mathbf{M}^{(u)}_q \\ -\mathbf{L}^{(u)}_q \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{c}_q \\ \begin{bmatrix} \mathbf{d}_q \\ \begin{bmatrix} \mathbf{c}_q \\ \mathbf{d}_q \end{bmatrix} \end{bmatrix} \end{bmatrix}. \] (5.43)

The matrices \( \mathbf{A}, \mathbf{B}, \mathbf{L}^{(u)}_q, \mathbf{M}^{(u)}_q, \mathbf{L}^{(v)}_q, \mathbf{M}^{(v)}_q \) represent the matrix elements of the GGPE and the BdGEs respectively, and are defined in appendix C.2.1. In the laboratory (LAB) frame in the axially symmetric case and in the absence of any vortices, we have \( \mathbf{L}^{(u)}_q = \mathbf{L}^{(v)}_q \) and \( \mathbf{M}^{(u)}_q = \mathbf{M}^{(v)}_q \), but this is not the case in general.

### 5.3.1 Numerical Solutions for the Quasi-2D BEC

In all cases, we assume axial symmetry of the confining potential. We also assume tight axial confinement \( (\omega_r \gg \omega_z) \) such that we can ignore all excitations in the axial direction, thus allowing the \( z \)-coordinate to be integrated out, yielding the 2D time-independent orthogonal HFB equations comprising the 2D time-independent GGPE (5.36) and the 2D time-independent orthogonal BdGEs (5.37). In the rotating frame the angular precessional frequency for off-axis vortices may be calculated using equation (4.65). We now consider the cases of no vortices, a single on-axis vortex, and of one or more off-axis vortices. In all cases we expand the condensate wave-function \( \Phi(r, \theta) \) and the quasi-particle amplitudes \( u_q(r_1, \theta_1) \) and \( v_q(r_1, \theta_1) \) in terms of the single-particle basis functions \( \xi_{ln}(r, \theta) \) satisfying the single-particle Schrödinger equation

\[ \mu^{(SP)}_{ln}(r, \theta) = \hat{h}(r, \theta)\xi_{ln}(r, \theta). \] (5.44)

These are simply the Laguerre basis functions \( \{ \xi_{ln}(r, \theta), l = 0, \pm 1, \ldots, n = 0, 1, \ldots \} \) defined by (C.26)

\[ \xi_{ln}(r, \theta) = \xi_{ln}(r) \frac{e^{i \theta}}{\sqrt{2\pi}} \] (5.45)

where the radial Laguerre function is given by

\[ \xi_{ln}(r) = \left( \frac{2n!}{(n + |l|)!} \right)^{1/2} e^{-r^2/2} r^{|l|} L_n^{|l|}(r^2) \] (5.46)

and where the \( L_n^{|l|}(r^2) \) are \( n \)th order modified Laguerre polynomials in \( r^2 \).

#### Axially-symmetric Solutions

In the case of axial symmetry of the solutions, we can integrate out the azimuthal coordinate \( \theta \) (see also section 7.2, chapter 7 and section C.2.2 of the appendix) to obtain the radial
time-independent orthogonal HFB equations comprised of the radial time-independent GGPE
\[
\Delta \mu \Phi(r) = \left( \hat{h}_{m,\Omega}(r) - \mu + C_{2D}^{R} (|\Phi(r)|^2 + 2\bar{n}(r)) \right) \Phi(r) + C_{2D}^{R} \bar{m}(r) \Phi(r) - \int_{0}^{\infty} r' dr' \hat{P}(r', r) \phi(r')
\]
(5.47)
and the radial time-independent orthogonal BdGEs
\[
\epsilon_{lq} \begin{bmatrix} u_{lq}(r) \\ v_{lq}(r) \end{bmatrix} = \int_{0}^{\infty} r' dr' \begin{bmatrix} Q_{l}(r, r') \hat{L}_{l+m}(r') & Q_{l}(r, r') \mathcal{M}(r') \\ -Q_{l}(r, r') \mathcal{M}(r') & -Q_{l}(r, r') \hat{L}_{l-m}(r') \end{bmatrix} \begin{bmatrix} u_{lq}(r') \\ v_{lq}(r') \end{bmatrix},
\]
(5.48)
where we have defined the radial operators \( \hat{L}_{l}(r) \), \( \mathcal{M}(r) \)
\[
\hat{L}_{l}(r) = \hat{h}_{l}(r) - \mu + 2C_{2D}^{R} (|\Phi(r)|^2 + \bar{n}(r))
\]
(5.49)
and by \( \hat{P}(r', r) \)
\[
\hat{P}(r', r) = (\bar{n}(r', r) \hat{L}(r') + \bar{m}(r', r) \mathcal{M}(r')) / \sqrt{N_{c}(t)}
\]
(5.50)
with the single-particle Hamiltonian in the LAB frame given by
\[
\hat{h}_{l}(r) = -\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{l^2}{r^2} - \mu + r^2,
\]
(5.51)
and by
\[
\hat{h}_{l,\Omega}(r) = -\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{l^2}{r^2} - l\Omega + r^2
\]
(5.52)
in the rotating frame. The radial projection operator \( Q(r, r_{1}) \) is given by
\[
Q_{l}(r, r') = \delta(r, r') - \delta_{l,0} \phi(r) \phi(r')
\]
(5.53)
and the radial 2D nonlinearity constant \( C_{2D}^{R} \equiv C_{2D} / 2\pi \) by
\[
C_{2D}^{R} = 4 \left( \frac{\lambda}{2\pi} \right)^{1/2} \frac{a_{s}}{r_{0}} N.
\]
(5.54)
In this case we can expand the radial condensate wave-function \( \Phi(r) \) and the radial quasi-particle amplitudes \( u_{lq}(r) \) and \( v_{lq}(r) \) in terms of the radial Laguerre basis functions \( \xi_{ln}(r) \), i.e.
\[
\Phi(r) = \sum_{n} a_{0,nn} \xi_{mn}(r)
\]
(5.55)
for the condensate wave-function, and
\[
u_{lq}(r) = \sum_{ln} c_{q,ln} \xi_{l+m,n}(r)
\]
(5.56)
and

\[ v_q(r) = \sum_{l,m,n} d_{q,l,m,n}(r) \]  

(5.57)

for the quasi-particle amplitudes. Here we have allowed for the existence of an on-axis vortex of vorticity \( m \). In the case of no vortices, \( m = 0 \). Thus we obtain the vector eigenvalue equation for the coefficients for the condensate wavefunction (GGPE) and for the quasiparticle amplitudes (BdGEs) given respectively by equations of the form (5.42) and (5.43) as before (see appendix C.2.2). We note that the radial Laguerre basis functions \( \xi_{ln}(r) \) given by equation (5.46) may be written as a polynomial of order \( n + l \) in \( r^2 \) times a weighting factor \( \exp(-r^2/2) \), thus all matrix elements are integrals of orthogonal polynomials of order \( 4N + 2M - 4 \) in \( r^2 \) (since \( dr^2 = 2rdr \)), where we have imposed the computational mode cut-off of \( n = 0, \ldots, N - 1 \) and \( l = 0, \pm 1, \ldots, \pm M \). This facilitates the use of Gaussian quadrature for the integration (see section (5.5)), allowing accurate computation for a minimal number of position points, greatly enhancing the efficiency and accuracy of the numerical algorithms used here.

**Single Off-axis Vortex**

We find stationary solutions for a single off-axis vortex by solving the 2D orthogonal HFB equations (5.36) and (5.37), and the equation for the precessional frequency (4.65) self-consistently with \( C(r, \theta) \) given by (4.125). We can write the condensate wave function \( \Phi(r, \theta) \) in in the Laguerre basis \( \{\xi_{ln}(r, \theta)\} \)

\[ \Phi(r, \theta) = \sum_{ln} a_{ln} \xi_{ln}(r, \theta) \]  

(5.58)

and similarly the quasi-particle amplitudes \( u_q(r, \theta) \), \( v_q(r, \theta) \)

\[ u_q(r, \theta) = \sum_{ln} c_{q,ln} \xi_{ln}(r, \theta) \]  

(5.59)

and

\[ v_q(r, \theta) = \sum_{ln} d_{q,ln} \xi_{ln}(r, \theta). \]  

(5.60)

Suppose we have a single vortex situated at position \( (r_1, \theta_1) \) such that \( (r_1, \theta_1) \) does not lie on any of the roots of the Laguerre basis functions \( \{\xi_{ln}(r, \theta)\} \). Then

\[ \Phi(r_1, \theta_1) = \sum_{ln} a_{ln} \xi_{ln}(r_1, \theta_1) = 0 \]  

(5.61)

so

\[ a_{10} = - \sum_{l,n \in S(1)} a_{ln} \frac{\xi_{ln}(r_1, \theta_1)}{\xi_{10}(r_1, \theta_1)} \]  

(5.62)
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gives the necessary constraint for the vortex to be at this position, where we have defined
\[ S^{(1)} \equiv \{ l, n \mid (l, n) \in S - \{(1, 0)\} \} \quad (5.63) \]
where \( S \equiv \{ l, n \mid n = 0, \ldots, l = 0, \pm 1, \ldots \} \) in anticipation of an iteration formula for the case of multiple vortices. Then we can write
\[
\Phi(r, \theta) = \sum_{l, n \in S^{(1)}} a_{ln} \chi_{ln}^{(1)}(r, \theta) \quad (5.64)
\]
where we have defined the modified basis functions
\[
\chi_{ln}^{(1)}(r, \theta) \equiv \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_1, \theta_1)}{\xi_{10}(r_1, \theta_1)} \xi_{10}(r, \theta) \quad (5.65)
\]
corresponding to a single vortex situated at \((r_1, \theta_1)\). Substituting (5.64) into the GGPE (5.36), and (5.59), (5.60) into the orthogonal BdGEs (5.37), and making use of the fact that
\[
\int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r, \theta) \chi_{ln}^{(1)}(r, \theta) = \delta_{l,l'} \delta_{n,n'} \quad (5.66)
\]
we again obtain the matrix equations for the coefficients for the condensate wavefunction (GGPE) and for the quasiparticle amplitudes (BdGEs) given by the vector equations of the form (5.42) and (5.43) (see appendix C.2.3).

Multiple Vortices

This procedure may be extended to \( N_v \) vortices situated at positions \((r, \theta) \in \{(r_i, \theta_i) \mid i = 1, \ldots N_v\}\) by an iterative process. Let us extend the notation (5.63) for \( N_v \) vortices, and define
\[
S^{(N_v)} \equiv \{ l, n \mid (l, n) \in S - \{(1, 0), \ldots, (N_v, 0)\} \}. \quad (5.67)
\]
Then suppose that for \( N_v - 1 \) vortices we can write
\[
\Phi(r, \theta) = \sum_{l, n \in S^{(N_v - 1)}} a_{ln} \chi_{ln}^{(N_v - 1)}(r, \theta) \quad (5.68)
\]
where the modified basis function for \( N_v - 1 \) vortices is given by
\[
\chi_{ln}^{(N_v - 1)}(r, \theta) \equiv \chi_{ln}^{(N_v - 2)}(r, \theta) - \frac{\chi_{ln}^{(N_v - 2)}(r_{N_v - 1}, \theta_{N_v - 1})}{\chi_{N_v - 1,0}^{(N_v - 2)}(r_{N_v - 1}, \theta_{N_v - 1})} \chi_{N_v - 1,0}^{(N_v - 2)}(r, \theta) \quad (5.69)
\]
Then introducing another vortex \( N_v \) at position \((r_{N_v}, \theta_{N_v})\) implies
\[
\Phi(r_{N_v}, \theta_{N_v}) = \sum_{l, n \in S^{(N_v)}} a_{ln} \chi_{ln}^{(N_v)}(r_{N_v}, \theta_{N_v}) = 0
\]
hence
\[ a_{Nv-1,0} = - \sum_{l,n \in S^{(Nv-1)}} a_{ln} \frac{\chi^{(Nv-1)}_{ln}(r_{Nv}, \theta_{Nv})}{\chi^{(Nv-1)}_{00}(r_{Nv}, \theta_{Nv})} \]
so that for \( Nv \) vortices
\[ \Phi(r, \theta) = \sum_{l,n \in S^{(Nv)}} a_{ln} \chi^{(Nv)}_{ln}(r, \theta) \]
where we define the modified basis functions
\[ \chi^{(Nv)}_{ln}(r, \theta) \equiv \chi^{(Nv-1)}_{ln}(r, \theta) - \frac{\chi^{(Nv-1)}_{ln}(r_{Nv}, \theta_{Nv})}{\chi^{(Nv-1)}_{00}(r_{Nv}, \theta_{Nv})} \chi^{(Nv-1)}_{00}(r, \theta) \]
for \( Nv \) vortices situated at \((r, \theta) \in \{(r_i, \theta_i) | i = 1, \ldots Nv\}\). Further it can be shown that
\[ \int_0^{2\pi} \int_0^{\infty} r dr d\theta \xi^{*}_{ln}(r, \theta) \chi^{(Nv)}_{ln}(r, \theta) = \delta_{ll'} \delta_{nn'} \]
permitting us to write the vector equations for the coefficients for the condensate wavefunction (GGPE) and for the quasiparticle amplitudes (BdGEs) in the form given respectively by equations (5.42) and (5.43) as before (see appendix C.2.3).

**Numerical Calculation of the Precessional Frequency \( \Omega \)**

We use equation (4.65) with \( C(r, \theta) \) given by (4.125) to calculate the precessional frequency \( \Omega \) in the case of single and multiple off-axis vortices. Let \( R = \text{Re} \{ \Phi \} \) and \( I = \text{Im} \{ \Phi \} \) represent respectively the real and imaginary parts of the condensate wavefunction, then
\[ \Phi(r, t) = R(r, t) + iI(r, t). \]
Calculation of the precessional frequency \( \Omega \) requires numerical computation of the quantities \( r \frac{\partial}{\partial r} \Phi(r, \theta), r^2 \frac{\partial^2}{\partial r^2} \Phi(r, \theta), \frac{\partial}{\partial \theta} \Phi(r, \theta), \) and \( \frac{\partial^2}{\partial \theta^2} \Phi(r, \theta) \) involving first and second order derivatives of the condensate function \( \Phi \) given by equations (C.115)-(C.118). The derivatives of the modified basis functions are found analytically using the recurrence relations of the Laguerre basis functions, and the iterative relations (5.65) and (5.70) for the modified basis functions for single and multiple vortices. This permits accurate computation of the derivatives (C.115)-(C.118), in contrast to numeric differentiation which would be very inaccurate for the Gaussian grid used here, and which would be very sensitive to numerical noise.

Using the recurrence relation [103, 104]
\[ r \frac{dL_n^k(r)}{dr} = nL_n^k(r) - (n + k)L_{n-1}^k(r) \]
for the generalised associated Laguerre polynomial $L_n^k(r)$, and the expression (5.46) for the radial Laguerre basis function $ξ_{ln}(r) = N_n^{|l|} e^{-r^2/2} r^{|l|} L_n^{|l|}(r^2)$, we find that

$$r \frac{dξ_{ln}(r)}{dr} = (2n + |l| - r^2) ξ_{ln}(r) - 2 \sqrt{n(n + |l|)} ξ_{l,n-1}(r)$$  \hspace{1cm} (5.74)$$

and

$$r^2 \frac{d^2ξ_{ln}(r)}{dr^2} = (2n + |l| - 1 - r^2) r \frac{dξ_{ln}(r)}{dr} - 2r^2 ξ_{ln}(r) - 2 \sqrt{n(n + |l|)} r \frac{dξ_{l,n-1}(r)}{dr}. \hspace{1cm} (5.75)$$

By (5.45) we have

$$\frac{\partial ξ_{ln}(r, θ)}{\partial θ} = ilξ_{ln}(r, θ)$$  \hspace{1cm} (5.76)$$

and

$$\frac{\partial^2 ξ_{ln}(r, θ)}{\partial θ^2} = -l^2 ξ_{ln}(r, θ). \hspace{1cm} (5.77)$$

This allows us to calculate the derivatives of the basis functions, and hence of the modified basis functions analytically. For a single vortex, the quantities $r \frac{\partial}{\partial r} χ_{ln}^{(1)}(r, θ), r^2 \frac{\partial^2}{\partial r^2} χ_{ln}^{(1)}(r, θ), \frac{\partial}{\partial θ} χ_{ln}^{(1)}(r, θ)$ and $\frac{\partial^2}{\partial θ^2} χ_{ln}^{(1)}(r, θ)$ for the modified Laguerre basis functions are given by equations (C.124)-(C.127). By a process of iteration one can calculate the derivatives in the case of any number of vortices $N_v$ by use of the equations (C.128)-(C.131) which follow directly from the iterative formula (5.70).

These derivatives for the modified Laguerre basis functions are pre-calculated (as are all basis functions used in these calculations), thus greatly enhancing performance.

### 5.4 Numerical Solution of the Time-dependent HFB Equations

We discuss two methods here for the solution of the time-dependent orthogonal HFB equations. The first method is the fourth-order Runge-Kutta interaction-picture (RK4IP) algorithm that uses fast Fourier transforms and inverse transforms, and the fourth-order Runge-Kutta numerical integration algorithm to solve the HFB equations in the interaction picture. The second is an algorithm where the wave-function and quasi-particle amplitudes are represented in the Laguerre basis, and a fourth-order Runge-Kutta algorithm used to determine the time evolution of the condensate wave-function and the quasi-particle amplitude coefficients.
5.4.1 Brief Description of the RK4IP Algorithm [90]

We consider a matrix differential equation of the form

\[ \frac{\partial \Psi(r, t)}{\partial t} = D\Psi(r, t) + G(\Psi(r, t), r, t)\Psi(r, t) \]  

(5.78)

where \( \Psi(r, t) \) is a vector wave function, \( D \) is a matrix differential operator with characteristic equation \( d(\alpha) \) (e.g. for \( D = \nabla^2 \), \( d(-2\pi i k) = |-2\pi i k|^2 \)), and \( G(\Psi(r, t), r, t) \) a matrix function of the vector wave-function \( \Psi(r, t) \), and of position \( r \) and time \( t \). We shall see presently how the time-dependent HFB equations can be cast in this form. We define the interaction picture wavefunction vector \( \Psi^I(r, t) \) given by

\[ \Psi^I(r, t) = \exp (-D(t - \xi)) \Psi(r, t) \]  

(5.79)

Then

\[ \frac{\partial \Psi^I(r, t)}{\partial t} = \exp (-D(t - \xi)) G(\Psi(r, t), r, t)\Psi(r, t) = f (\Psi^I(r, t), r, t) \]  

(5.80)

where we define the vector function

\[ f (\Psi^I(r, t), r, t) = \exp (-D(t - \xi)) G(\Psi(r, t), r, t)\Psi(r, t) \]  

(5.81)

for some arbitrary parameter \( \xi \), which we will choose later in such a way as to optimise the algorithm. Using the fourth order Runge-Kutta algorithm (see for example [91]), we integrate this equation numerically. The value of \( \Psi^I(r, t) \), the vector wavefunction in the interaction picture at the \((n + 1)\)th step is given by

\[ \Psi^I(r, t_{n+1}) = \Psi^I(r, t_n) + \frac{[k_1 + 2 (k_2 + k_3) + k_4]}{6} \]  

(5.82)

where

\[ k_1 = f (\Psi^I(r, t_n), r, t_n) \Delta t \]  

(5.83)

\[ k_2 = f \left( \Psi^I(r, t_n + \frac{\Delta t}{2}) + \frac{k_1}{2}, r, t_n + \frac{\Delta t}{2} \right) \Delta t \]  

(5.84)

\[ k_3 = f \left( \Psi^I(r, t_n + \frac{\Delta t}{2}) + \frac{k_2}{2}, r, t_n + \frac{\Delta t}{2} \right) \Delta t \]  

(5.85)

\[ k_4 = f (\Psi^I(r, t_n + \Delta t) + k_3, r, t_n + \Delta t) \Delta t \]  

(5.86)

where we have defined the function \( f (\Psi^I(r, t), r, t) \) as above (5.81). This Runge-Kutta step advances \( \Psi^I(r, t_n) \) \( \rightarrow \) \( \Psi^I(r, t_{n+1}) \). We can evaluate \( f (\Psi^I(r, t), r, t) \) from (5.81) using the Fourier transform technique, we find that

\[ f (\Psi^I(r, t), r, t) = \mathcal{F}_k^{-1} \{ \mathcal{F}_r \{ G(\Psi(r, t), r, t)\Psi(r, t) \} \exp (-d(-2\pi i k)(t - \xi)) \} \]  

(5.87)
where \( G(k, f) \equiv \mathcal{F}_r \{ g(r, t) \} \) represents the Fourier transform for some arbitrary vector function \( g(r, t) \), and \( \mathcal{F}_k^{-1} \{ G(k, f) \} = g(r, t) \) the inverse Fourier transform. Finally we use (5.79) to compute the vector wavefunction \( \Psi(r, t_{n+1}) \) at time step \( n+1 \)

\[
\Psi(r, t_{n+1}) = \exp(D(t_{n+1} - \xi_{n+1})) \Psi^I(r, t_{n+1}). \tag{5.88}
\]

Let us choose

\[
\xi_n = t_n + \Delta t/2 \tag{5.89}
\]

This minimises the number of Fourier transform operations required (see [90]). Defining the following operators

\[
\mathcal{D}(\Psi) = \exp \left( \frac{\Delta t}{2} D \right) \Psi \tag{5.90}
\]

and

\[
\mathcal{G}(\Psi, t) = \Delta t G(\Psi, t) \Psi \tag{5.91}
\]

where \( g \) requires \( k \) in the normal picture (i.e. not in the interaction picture). The algorithm may be summarised as follows\(^2\) (see [90]) :

\[
\Psi^I \leftarrow \mathcal{D}(\Psi) \quad \quad \quad \quad \leftarrow \Psi(r, t_n) \quad \text{input}
\]

\[
k_1 \leftarrow \mathcal{D}(\mathcal{G}(\Psi, t))
\]

\[
t \leftarrow t + \Delta t/2 \quad \quad \quad \text{time at midpoint}
\]

\[
k_2 \leftarrow \mathcal{G}(\Psi^I + k_1/2, t) \quad \quad \quad \text{Can use normal picture}
\]

\[
k_3 \leftarrow \mathcal{G}(\Psi^I + k_2/2, t) \quad \quad \quad \text{Can use normal picture}
\]

\[
t \leftarrow t + \Delta t/2 \quad \quad \quad \text{time at endpoint}
\]

\[
k_4 \leftarrow \mathcal{G}(\mathcal{D}(\Psi^I + k_3), t)
\]

\[
\Psi \leftarrow \mathcal{D}(\Psi^I + (k_1 + 2(k_2 + k_3))/6) + k_4/6 \quad \rightarrow \Psi(r, t_{n+1}) \quad \text{output}
\]

In this algorithm we are essentially calculating the wave-function (5.82) in the interaction picture\(^3\) and hence \( k_1 \) (equation (5.83)) at time \( t_n \) (second step), \( k_2 \) and \( k_3 \) at time \( t_n + \Delta t/2 \), and finally \( k_4 \) at time \( t_n + \Delta t \) according to equations (5.84)-(5.86) respectively. Finally we calculate the wave-function in the interaction picture at time \( t_n + \Delta t \) (equation (5.82)),

\(^2\)This algorithm requires just four Fourier transform operations per time step. The choice of \( \xi_n \) in (5.89) implies that we don’t need to convert to the interaction picture at time \( t + \Delta t/2 \) - we can just use the normal picture. Thus we can reduce the number of Fourier transform operations per time step from eight down to four.

\(^3\)Choosing \( \xi_n = t_n + \Delta t/2 \) in (5.90) at time \( t_n + \Delta t/2 \) implies that in the two derivative evaluations at the midpoint (i.e. in evaluating \( k_2 \) and \( k_3 \)), \( \exp(-D(t_n + \Delta t/2 - \xi_n)) \rightarrow 1 \), and therefore that there is no need to perform any Fourier transforms at this point, and also implies that we can use the normal picture at these points, since then \( \Psi^I = \Psi \) by equation (5.88).
and then transform back to the normal picture using equation (5.87) (final step). Since we have chosen \( \xi_n = t_n + \Delta t \) (equation (5.89)), we need only perform four Fourier transform operations per time step, namely in steps 1 and 2 (since \( \Psi_I \) and \( k_1 \) need to be in the interaction picture), \( k_4 \) which needs to be transformed back to the normal picture (step 7), and \( \Psi_I + (k_1 + 2(k_2 + k_3))/6 \) which also needs to be transformed back to the normal picture (final step). Note that \( k_4 \) is already in the normal picture.

5.4.2 Implementation of Time-dependent HFB using the RK4IP Algorithm

The time-dependent orthogonal dimensionless 2D HFB equations in the LAB frame in the interaction picture in Cartesian coordinates \( r = (x, y) \) are given by the time-dependent GGPE

\[
\frac{i}{\partial t} \Phi(r, t) = \left( \hat{h} - \mu + C_{2D} (|\Phi|^2 + 2\bar{n}) \right) \Phi(r, t) + C_{2D} \bar{m} \Phi^*(r, t) - \int d r' \hat{P}(r', r, t) \phi(r', t) + C_{2D} \bar{m} \Phi(r, t)
\]

and the time-dependent BdGEs

\[
\frac{i}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \int d r' \begin{bmatrix} \hat{L}(r, r', t, -\epsilon_q) & \mathcal{M}(r, r', t) \\ -\mathcal{M}^*(r, r', t) & -\hat{L}^*(r, r', t, \epsilon_q) \end{bmatrix} \begin{bmatrix} u_q(r', t) \\ v_q(r', t) \end{bmatrix}
\]

where

\[
\hat{L}(r, r', t, \epsilon_q) \equiv \hat{L}(r, r', t) + \epsilon_q \delta(r - r')
\]

and

\[
\hat{L}(r, r', t, \epsilon_q) \equiv \hat{L}(r, r', t) + \epsilon_q \delta(r - r')
\]

where we have neglected \( \Delta \mu \) (see section 4.2.3, chapter 4). For standard HFB\(^4\) (i.e. \( \hat{P}(r, r') = 0 \) and \( Q(r, r', t) = \delta(r, r') \)). Thus the GGPE (5.92) can be written in the form

\[
\frac{\partial \Phi}{\partial t} = \mathbf{D} \Phi + \mathbf{G}_\Phi \Phi
\]

where

\[
\Phi \equiv \begin{bmatrix} \Phi \\ \Phi^* \end{bmatrix},
\]

\[
\mathbf{D} \equiv i \begin{bmatrix} \nabla^2 & 0 \\ 0 & -\nabla^2 \end{bmatrix},
\]

and

\[
\mathbf{G}_\Phi \equiv -i \begin{bmatrix} V_T - \mu + C_{2D} (|\Phi|^2 + 2\bar{n}) & C_{2D} \bar{m} \\ -C_{2D} \bar{m}^* & -(V_T - \mu + C_{2D} (|\Phi|^2 + 2\bar{n})) \end{bmatrix}
\]

\(^4\)We note that the RK4IP algorithm given here is only valid for the standard time-dependent HFB formalism.
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and the BdGEs (5.93) as
\[ \frac{\partial w_q}{\partial t} = D w_q + G_{uv} w_q \] (5.99)

where
\[ w_q \equiv \begin{bmatrix} u_q \\ v_q \end{bmatrix} \] (5.100)

and
\[ G_{uv} \equiv -i \begin{bmatrix} V_T - \epsilon_q + 2C_{2D} (|\Phi|^2 + \bar{n}) & C_{2D} (\Phi^2 + \bar{m}) \\ -C_{2D} (\Phi^2 + \bar{m}^*) & - (V_T + \epsilon_q + 2C_{2D} (|\Phi|^2 + \bar{n})) \end{bmatrix}. \] (5.101)

Each of these equations is of the form
\[ \frac{\partial \Psi(r, t)}{\partial t} = D \Psi(r, t) + G(\Psi(r, t), r, t) \Psi(r, t) \] (5.102)
as in (5.78) above.

5.4.3 Implementation of Time-dependent HFB using RK4 Algorithm for evolution of Coefficients

The problems with the RK4IP algorithm may be summarised as follows:

1. The BdGEs need to be solved for each mode. This requires a considerable amount of memory for a reasonable energy cut-off.

2. The RK4IP algorithm uses a Fourier grid. This imposes considerable limitations on the resolution of the vortex core, since the mesh must be uniform.

We propose an algorithm here in which the condensate wavefunction and quasiparticle amplitudes are expanded in terms of the Laguerre basis functions, requiring the calculation of matrix elements at each time step. Thus one obtains a first order differential equation in time for the coefficients for the condensate wavefunction, and the quasiparticle amplitudes. Use of a Gaussian grid drastically reduces the overhead of calculation of the matrix elements. The advantages of this algorithm are as follows:

1. A dramatic reduction in memory is achieved, thus the energy cut-off can be substantially increased.
2. The algorithm is grid independent, since it is the coefficients that are calculated, not the wavefunction and quasiparticle amplitudes themselves. The Gaussian grid is used merely to evaluate the matrix elements required in these calculations. Thus the display grid is arbitrary, hence the core region can be accurately represented.

3. Since the Gaussian grid is considerably smaller than the Fourier grid, the computations for a given energy cut-off are substantially faster.

4. The aliasing effects associated with Fourier transforms are avoided.

5. The algorithm is extendable to the orthogonal formalism.

Let us consider the quasi-2D case. We expand the condensate wavefunction $\Phi(r, \theta, t)$ and quasiparticle amplitudes $u_q(r, \theta, t), v_q(r, \theta, t)$ in the Laguerre basis $\{\xi_{ln}(r, \theta)\}$ (see appendix C.3.3)

$$\Phi(r, \theta, t) = \sum_{ln} a_{0,ln}(t) \xi_{ln}(r, \theta) \quad (5.103)$$

$$u_q(r, \theta, t) = \sum_{ln} c_{ln}(t) \xi_{ln}(r, \theta) \quad (5.104)$$

and

$$v_q(r, \theta, t) = \sum_{ln} d_{ln}(t) \xi_{ln}(r, \theta) \quad (5.105)$$

where the Laguerre basis functions are given by (5.45). Substituting (5.103) into the GGPE (5.92), and (5.104),(5.105) into the orthogonal BdGEs (5.93) in the interaction picture, we obtain the vector equations

$$i \frac{d\mathbf{a}(t)}{dt} = \mathbf{Aa}(t) + \mathbf{Ba}^*(t) \quad (5.106)$$

for the evolution of the coefficients for the condensate wave-function (GGPE), and

$$i \frac{d\mathbf{c}_q(t)}{dt} \begin{bmatrix} \mathbf{c}_q(t) \\ \mathbf{d}_q(t) \end{bmatrix} = \begin{bmatrix} \mathbf{L}_q^{(u)} & \mathbf{M}_q^{(u)} \\ -\mathbf{M}_q^{(v)} & -\mathbf{L}_q^{(v)} \end{bmatrix} \begin{bmatrix} \mathbf{c}_q(t) \\ \mathbf{d}_q(t) \end{bmatrix} \quad (5.107)$$

for the quasiparticle amplitudes (BdGEs), where $\mathbf{a}, \mathbf{c}_q$ and $\mathbf{d}_q$ are the vectors corresponding to the coefficients $a_{ln}, c_{q,ln}$ and $d_{q,ln}$, and $\mathbf{A}, \mathbf{B}, \mathbf{L}_q^{(u)}, \mathbf{M}_q^{(u)}, \mathbf{L}_q^{(v)}$ and $\mathbf{M}_q^{(v)}$ the matrices corresponding to the matrix elements $A_{ln,l'n'}, B_{ln,l'n'}, L_{ln,l'n'}^{(u)}, M_{ln,l'n'}^{(u)}, L_{ln,l'n'}^{(v)}$ and $M_{ln,l'n'}^{(v)}$. Each of the above matrix equations can be re-written in the form

$$\frac{d\chi(t)}{dt} = \mathbf{f}(\chi(t), t) \quad (5.108)$$

where $\mathbf{f}(\chi(t), t)$ is a vector function of the form

$$\mathbf{f}(\chi(t), t) = \mathbf{F}\chi(t) \quad (5.109)$$
for some matrix $F$. In the case of the dynamical equation for the evolution of the coefficients $a(t)$ for the condensate wave-function (GGPE), we can re-write equation (5.106) as

$$\frac{d}{dt}\begin{bmatrix} a(t) \\ a^*(t) \end{bmatrix} = \frac{1}{i} \begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix} \begin{bmatrix} a(t) \\ a^*(t) \end{bmatrix}$$

(5.110)

which is of the required form.

We can integrate the vector equation (5.108) using the standard fourth-order Runge-Kutta algorithm, thus

$$f(\chi(t_{n+1}), t_{n+1}) = f(\chi(t_n), t_n) + \frac{k_1 + 2(k_2 + k_3) + k_4}{6}$$

(5.111)

where

$$k_1 = f(\chi(t_n), t_n) \Delta t$$

(5.112)

$$k_2 = f\left(\chi(t_n + \frac{\Delta t}{2}) + \frac{k_1}{2}, t_n + \frac{\Delta t}{2}\right) \Delta t$$

(5.113)

$$k_3 = f\left(\chi(t_n + \frac{\Delta t}{2}) + \frac{k_2}{2}, t_n + \frac{\Delta t}{2}\right) \Delta t$$

(5.114)

$$k_4 = f(\chi(t_n + \Delta t) + k_3, t_n + \Delta t) \Delta t.$$  

(5.115)

**Verification of Kohn’s Theorem** Preliminary time-independent simulations using both the RK4IP and the RK4 algorithm for the evolution of the coefficients (not presented here) verify that Kohn’s theorem is rigorously observed in both cases, as are the number and angular momentum conservation laws.

**Use of Orthogonal Formalism** The results obtained using the standard and the orthogonal time-dependent HFB formalisms are qualitatively very similar. This was verified in several simulations, but owing to the extra computational effort required in calculating the projection part $\int d\mathbf{r}' \hat{P}(\mathbf{r}', \mathbf{r}, t) \phi(\mathbf{r}', t)$ in the orthogonal GGPE (5.92) the standard time-dependent HFB algorithm was used for all of the simulations presented here - see footnote at the start of section 5.1.

### 5.5 Gaussian Quadrature

Gaussian quadrature is an integration technique that provides very accurate integration for a minimal number of grid points. It is applicable to integrands that may be written as
the product of a polynomial of order \(2N - 1\) times a weighting function, i.e. in evaluating integrals of the form

\[
\int_{b}^{a} w(x) P_{2N-1}(x) dx
\]  

(5.116)

where the \(P_{2N-1}(x)\) is a polynomial of order \(2N - 1\) in \(x\) and \(w(x)\) is a weighting function in \(x\) defined over the closed interval \([a, b]\). Let \(\{f_n(x)\}\) be a sequence of orthogonal polynomials of order \(n\) in \([a, b]\) relative to the weighting function \(w(x)\). Then it can be shown that \([91]\)

\[
\int_{b}^{a} w(x) P_{2N-1}(x) dx = \sum_{k=1}^{N} \alpha_k P_{2N-1}(x_k)
\]  

(5.117)

where the constants \(\alpha_k\) are given by

\[
\alpha_k = \int_{a}^{b} w(x) L_k(x) dx
\]  

(5.118)

with

\[
L_k = \frac{\prod_{i \neq k}(x - x_i)}{\prod_{i \neq k}(x_k - x_i)}
\]  

(5.119)

where the \(\{x_k, k = 1, 2, \ldots, N\}\) are the zeros of \(f_n(x) = 0\).

This shows that the integration is exact for polynomials up to order \(2N - 1\), given a sequence \(\{f_n(x)\}\) of orthogonal polynomials. Often the integration accuracy is very good for polynomials of order greater than \(2N - 1\) provided \(N\) is sufficiently large. Well-behaved functions can also be approximated by the representation \(w(x) P_{2N-1}(x)\).

Here the wave-functions and the quasi-particle amplitudes are expanded in the Laguerre basis, hence defining \(\rho = r^2\) and noting that \(d\rho = dr^2 = 2rdr\), we see that all radial densities can be written in the form \(\exp(-\rho) P_{2N+L-2}(\rho)\), and all radial matrix products in the form \(\exp(-\rho) P_{4N+2L-4}(\rho)\), so we need \(2N + L\) radial grid points to evaluate radial matrix densities to machine precision. Regarding the azimuthal coordinate \(\theta\), we assume that the \(\theta\)-dependence is relatively smooth, and can therefore be well represented by a polynomial of order \(2K - 1\) with weighting factor \(w(x) = 1\), and the integrals accurately evaluated for a grid of \(K\) azimuthal grid points using the sequence of Legendre orthogonal polynomials.

In most of the integrations performed here, \(N_r = 41\) radial points and \(N_\theta = 40\) azimuthal points were used (a grid of \(41 \times 40\) points), though in certain circumstances involving several vortices or in cases of vigorous stirring or trap axial symmetry-breaking it was necessary to use \(N_r = 61\) and \(N_\theta = 60\) for accurate integration.
5.6 Computational Accuracy and Mode Energy Cut-off

In view of the large number of calculations necessary, the numbers of computational modes and grid points were kept to a minimum whilst still maintaining reasonable computational accuracy ($\sim 1-2\%$). This was verified by doubling the number of computational modes in certain limited cases, and observing the change. Since the aim here is a proof in principle of the method of calculation of the precessional frequency and how this correlates with the LCLS energies, accuracy is not the main concern - only that reasonable accuracy is maintained, and that the solutions can be refined later, if required. In the calculations here, 209 computational modes were used corresponding to $n = 1, \ldots, 10$ and $l = 0, \pm 1, \ldots, \pm 10$, and the effect of doubling the number of computational modes found to be relatively small. Since Gaussian quadrature (see next section) was used for the radial integration, in most cases $N_r = 41$ was sufficient. In some cases involving multiple vortices, this number was increased to $N_r = 61$. Gaussian quadrature was also used for the azimuthal ($\theta$) integration by use of the Legendre orthogonal polynomials, and provided the change in angular dependence is not too rapid, $N_\theta = 40$ ensures good computational accuracy. In some cases involving multiple vortices, this number had to be increased to $N_\theta = 60$.

As we shall see in chapter 7, a mode cut-off of $N_m = 100$ is sufficient for most vortex precession calculations. This is not sufficient for the perturbation calculations (not presented here). In these preliminary calculations, we find that the shifts in the quasi-particle excitation energies have a relatively small effect on the thermal and anomalous densities, and therefore we would expect the effects on the vortex precession results to be insignificant. Since the extra computational overhead in the self-consistent calculations for the vortex precession calculations is significant, the orthogonal time-independent HFB equations are solved self-consistently with the precessional frequency prediction calculations without the extra overhead of the self-consistent perturbation calculations.

5.7 Vortex Detection and Tracking Algorithm

5.7.1 Vortex Detection

The vortex detection algorithm is the same as that used by B. M. Caradoc-Davies in his PhD Thesis [90]. For each point (excluding the grid points on the boundary) a detection
grid is set up as shown in figure 5.1 which shows the case of a positive vortex characterised by a phase-flow in the anti-clockwise direction, and represented by the symbol + indicating a singly-charged vortex.

Let us define the quantity \( U(\alpha, \beta) \) by

\[
U(\alpha, \beta) = \begin{cases} 
-1 & \text{if } \beta - \alpha > \pi \\
0 & \text{if } -\pi \leq \beta - \alpha \leq \pi \\
1 & \text{if } \beta - \alpha < -\pi 
\end{cases}
\] (5.120)

and the set of pairs of wave-function phase angles \( A_{ij} \) by

\[
A_{ij} = \{ (\phi_1, \phi_2), (\phi_2, \phi_3), \ldots, (\phi_7, \phi_8), (\phi_8, \phi_1) \} 
\] (5.121)

where the \( \phi_i \) are short-hand representations for the phase-angles

\[
\begin{align*}
\phi_1 & \equiv \text{arg} (\Phi_{i-1,j-1}) \\
\phi_2 & \equiv \text{arg} (\Phi_{i,j-1}) \\
\phi_3 & \equiv \text{arg} (\Phi_{i+1,j-1}) \\
\phi_4 & \equiv \text{arg} (\Phi_{i+1,j}) \\
\phi_5 & \equiv \text{arg} (\Phi_{i+1,j+1}) \\
\phi_6 & \equiv \text{arg} (\Phi_{i,j+1}) \\
\phi_7 & \equiv \text{arg} (\Phi_{i-1,j+1}) \\
\phi_8 & \equiv \text{arg} (\Phi_{i-1,j}) 
\end{align*}
\] (5.122)

We then define the vortex detection array by

\[
V_{ij} = \sum_{(\alpha, \beta) \in A_{ij}} U(\alpha, \beta). 
\] (5.123)

\( V_{ij} = +1 \) indicates a vortex of charge +1 at position \((i, j)\) on the grid, and -1 a vortex of charge -1. The density curvature at point \((i, j)\) is given by

\[
\kappa = \frac{|\Phi_{i-1,j}|^2 + |\Phi_{i+1,j}|^2 - 2 |\Phi_{i,j}|^2}{(\Delta x)^2} + \frac{|\Phi_{i,j-1}|^2 + |\Phi_{i,j+1}|^2 - 2 |\Phi_{i,j}|^2}{(\Delta y)^2}. 
\] (5.124)

We set up a threshold \( \kappa_\nu \) for the detection of vortices, and neglect vortices in low density regions of the condensate, i.e. for \( \kappa < \kappa_\nu \). Here we choose \( \kappa \sim 10^{-1} \) since we wish only to track vortices in regions of appreciable density in our stirring and trap axial symmetry-breaking simulations in order to limit the number of vortex tracks, though this can be easily changed if necessary.
5.7.2 Vortex Tracking

Once a vortex is detected, an index reference and an acquisition window is set up for the vortex. The position of the vortex is determined by setting up a refined grid defined by the acquisition window (which is possible in the case of the RK4 algorithm for the evolution of coefficients - another motivation for using this algorithm in preference to the RK4IP algorithm), and by finding the position of minimum density (which is theoretically zero, but which is in practice some small number depending on the coarseness of the grid). In this way accurate positions for the vortices may be determined. A track is set up for each vortex detected, and is terminated once that vortex becomes sub-threshold. Once the simulation is completed, the tracks can be matched up, and trajectories for each of the vortices plotted.
5.8 Presentation of Data where Time Evolution of HFB Equations is expressed in Coefficients

When using the RK4 algorithm above, one stores only the condensate wavefunction coefficients \( \{ a_{ln}(t) \} \) and the quasiparticle amplitude coefficients \( \{ c_{q,ln}(t) \} \) and \( \{ d_{q,ln}(t) \} \) for each time step in a file - i.e. the data is not grid dependent. Thus one is free to choose whatever grid is convenient, over any range desired. Here it is desirable to represent the data in Cartesian coordinates. The coefficients here are in the Laguerre representation. From a numerical viewpoint, it is more convenient to use the Hermite representation, since this is much more efficient numerically, as we will see presently. To do this, one must make a Laguerre to Hermite transformation of the coefficients. Then any Cartesian grid can be deployed.

**Laguerre-Hermite Transformation**  To do this one must first create a Hermite-Gaussian grid in the \( x \)- and \( y \)- coordinates. Then the condensate wavefunction is given by

\[
\Phi(x, y, t) = \sum_{ln} a_{ln}(t) \xi_{ln}(x, y)
\]

where

\[
\xi_{ln}(x, y) = \left( \frac{n!}{\pi (n + |l|)!} \right)^{1/2} e^{-x^2 + y^2/2} L_n^{|l|}(x^2 + y^2) (x + i \text{sgn}(l) y)^{|l|}
\]

where \( L_n^{|l|} \) is a modified Laguerre polynomial of order \( n \), and where

\[
\text{sgn}(l) \equiv \begin{cases} 
1 & \text{if } l \geq 0 \\
-1 & \text{if } l < 0.
\end{cases}
\]

The Hermite basis set is given by \( \{ \zeta_n(x) \} \) where

\[
\zeta_n(x) = \left( \frac{1}{\sqrt{\pi} 2^{n} n!} \right)^{1/2} e^{-x^2/2} H_n(x)
\]

where \( H_n(x) \) is a Hermite polynomial of order \( n \). We can express \( \Phi(x, y, t) \) in terms of Hermite basis functions by writing

\[
\Phi(x, y, t) = \sum_{mn} b_{mn}(t) \zeta_m(x) \zeta_n(y)
\]

We can determine the coefficients \( \{ b_{mn}(t) \} \) in terms of the \( \{ a_{ln}(t) \} \) coefficients as follows. We first note by the orthonormality properties of the Hermite basis functions that

\[
b_{mn}(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy \zeta_m^*(x) \zeta_n^*(y) \Phi(x, y, t) = \sum_{l'n'} a_{l'n'}(t) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy \zeta_m^*(x) \zeta_{n'}^*(y) \xi_{l'n'}(x, y).
\]
Thus we can transform from the Laguerre representation into the Hermite representation using the transformation

\[ b_{mn}(t) = \sum_{l'n'} a_{l'n'}(t) A_{mn, l'n'} \]

(5.131)

where

\[ A_{mn, l'n'} \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy \zeta_m^*(x) \zeta_n^*(y) \xi_{l'n'}(x, y). \]

(5.132)

One can represent this as a matrix transformation

\[ \mathbf{b}(t) = \mathbf{Aa}(t) \]

(5.133)

by defining the vectors \( \mathbf{a} \) and \( \mathbf{b} \), and the matrix \( \mathbf{A} \) by

\[
\begin{bmatrix}
\vdots \\
a_{-in}(t) \\
\vdots \\
a_{in}(t)
\end{bmatrix},
\begin{bmatrix}
b_{00}(t) \\
\vdots \\
b_{mn}(t) \\
\vdots \\
b_{N_m 0}
\end{bmatrix},
\begin{bmatrix}
\cdots & A_{00, -in} & \cdots & A_{00, in} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\cdots & A_{mn, -in} & \cdots & A_{mn, in} & \cdots
\end{bmatrix}
\]

(5.134)

Numerically, the Hermite representation is considerably more convenient. Let

\[
\chi \equiv \begin{bmatrix}
\zeta_0(x_0) & \cdots & \zeta_m(x_0) & \cdots & \zeta_{N_m}(x_0) \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
\zeta_0(x_n) & \cdots & \zeta_m(x_n) & \cdots & \zeta_{N_m}(x_n) \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
\zeta_0(x_{N_x}) & \cdots & \zeta_m(x_{N_x}) & \cdots & \zeta_{N_m}(x_{N_x})
\end{bmatrix}
\]

(5.135)

be a matrix of size \( (N_x \times N_m) \) where \( N_x \) represents the number of points in the 1D Cartesian Gaussian grid, and \( N_m \) the number of modes determined by some energy cut-off criterion, and

\[
\mathbf{B} \equiv \begin{bmatrix}
b_{00}(t) & \cdots & b_{0n}(t) & \cdots & b_{0N_m}(t) \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
b_{m0}(t) & \cdots & b_{mn}(t) & \cdots & b_{mN_m}(t) \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
b_{N_m 0}(t) & \cdots & b_{N_m n}(t) & \cdots & b_{N_m N_m}(t)
\end{bmatrix}
\]

(5.136)
Then the matrix representing the condensate wavefunction $\Phi(x, y, t_n)$ at time step $n$ defined by

$$
\Phi_n \equiv \begin{bmatrix}
\Phi(x_0, y_0, t_n) & \cdots & \Phi(x_0, y_j, t_n) & \cdots & \Phi(x_0, y_{N_x}, t_n) \\
\vdots & & \vdots & & \vdots \\
\Phi(x_i, y_0, t_n) & \cdots & \Phi(x_i, y_j, t_n) & \cdots & \Phi(x_i, y_{N_x}, t_n) \\
\vdots & & \vdots & & \vdots \\
\Phi(x_{N_x}, y_0, t_n) & \cdots & \Phi(x_{N_x}, y_j, t_n) & \cdots & \Phi(x_{N_x}, y_{N_y}, t_n)
\end{bmatrix}
$$

(5.137)

may be computed by pre- and post-multiplication, viz.

$$
\Phi_n = \chi B \chi^T
$$

(5.138)

One can do the same for the quasiparticle amplitudes using the same transformation, viz.

$$
e_q(t) = A c_q(t)$$

(5.139)

$$f_q(t) = A d_q(t)$$

where the quasiparticle amplitudes are now given by

$$
u_q(x, y, t) = \sum_{mn} e_{q,mn}(t) \zeta_m(x) \zeta_n(y)$$

(5.140)

and

$$
\nu_q(x, y, t) = \sum_{mn} f_{q,mn}(t) \zeta_m(x) \zeta_n(y).
$$

(5.141)

5.9 Concluding Remarks

In this chapter we presented the numerical algorithms for solving the time-independent and time-dependent orthogonal HFB equations. It is easy to modify these algorithms to implement standard HFB calculations. All time-independent calculations in this thesis were performed using the orthogonal HFB formalism. In the time-dependent case, however, this implies extra computation and smaller step size to maintain orthogonality to reasonable accuracy, therefore all the results presented here were performed using standard HFB. However, many time-dependent simulations have subsequently been repeated using the orthogonal HFB formalism, but the differences have been insignificant, and therefore have not been presented here to reduce on bulk of material.
Chapter 6

Simulation of Evaporative Cooling of Dilute Quasi-Two Dimensional BECs

6.1 Introduction

In this chapter, we implement a Gaussian out-coupler, and calculate the $g^{(2)}$ correlation function for the out-coupled beam. The purpose of this is firstly to test the functionality of the time-dependent algorithm, and secondly to simulate the cooling of a quasi-2D BEC by means of evaporative cooling. We perform time-dependent standard HFB calculations to simulate a cold dilute Bose gas undergoing evaporative cooling. We simulate the adiabatic cooling process by coupling atoms out of the BEC using a complex coupling potential in the form of an annulus having a Gaussian cross-sectional profile of starting radius well outside the Thomas-Fermi radius, and slowly diminishing this radius to a final radius still lying well outside the Thomas-Fermi radius. Since the thermal atoms lie farthest from the axis, and there are very few condensate atoms lying outside the Thomas-Fermi radius, we would expect the out-coupled atoms to be predominantly thermal atoms. This should provide significant cooling of the condensate. We carry out this procedure for various rates of cooling, and estimate the effective temperature of the BEC at various times during the cooling process. We establish the response time of the system, and to what degree the system equilibrates. However, it should be noted at the outset, that the Landau and Beliaev processes are missing in the HFB formalism, and therefore we would not expect to see re-thermalisation. Therefore we would not expect to see any condensate growth, and any cooling that takes place is due to removal of the high energy particles well outside the Thomas-Fermi radius.
6.2 Coherence Properties of an Out-coupled Beam of Atoms from a BEC [93, 94]

We consider an out-coupling potential $-iV_c(r, t)$. This gives us the GGPE

$$i\hbar \frac{\partial \Phi(r, t)}{\partial t} = \left( \hat{h}(r, t) - iV_c(r) - \mu + g \left( |\Phi(r, t)|^2 + 2\tilde{n}(r, t) \right) \right) \Phi(r, t) + g\tilde{m}(r, t)\Phi^*(r, t)$$

(6.1)

and the (non-orthogonal) BdGEs

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_p(r, t) \\ v_p(r, t) \end{bmatrix} = \begin{bmatrix} \hat{L}^{(C)}(r, t) - \epsilon_q & \mathcal{M}(r, t) \\ -\mathcal{M}^*(r, t) & -\left( \hat{L}^{(C)}(r, t) + \epsilon_q \right) \end{bmatrix} \begin{bmatrix} u_p(r, t) \\ v_p(r, t) \end{bmatrix}$$

(6.2)

in the interaction-picture, where we have defined the operator $\hat{L}^{(C)}(r, t)$ by

$$\hat{L}^{(C)}(r, t) \equiv \hat{L}(r, t) - iV_c(r, t).$$

(6.3)

Then the rate of change of condensate particles is given by

$$\frac{dN_c}{dt} = -\frac{2}{\hbar} \int dV_c(r)n_c(r) + i\frac{g}{\hbar} \int dr \left( \tilde{m}(r)\Phi^*(r) - \tilde{m}^*(r)\Phi(r) \right)$$

(6.4)

and the rate of change of the thermal population by

$$\frac{d\tilde{N}}{dt} = -\frac{2}{\hbar} \int dV_c(r)\tilde{n}(r) - i\frac{g}{\hbar} \int dr \left( \tilde{m}(r)\Phi^*(r) - \tilde{m}^*(r)\Phi(r) \right)$$

(6.5)

(see appendix B.2.1), where $N_c$ is the total number of condensate particles and $\tilde{N}$ the total number of thermal particles. Then if we define $N_{tot}$ to be the total number of particles in the BEC, we find that the rate at which particles are coupled out of the BEC is given by

$$\frac{dN_{tot}}{dt} = -\frac{2}{\hbar} \int dV_c(r, t)n_{tot}(r, t)$$

(6.6)

where $n_{tot} = n_c + \tilde{n}$. We note that in the absence of the out-coupling potential

$$\frac{dN_{tot}}{dt} = 0$$

(6.7)

hence the total number of particles is conserved.

We use the second-order coherence function [92]

$$g^{(2)}(r, r', t) = \frac{\left\langle \hat{\psi}^\dagger(r, t)\hat{\psi}^\dagger(r', t)\hat{\psi}(r', t)\hat{\psi}(r, t) \right\rangle}{\left\langle \hat{\psi}^\dagger(r, t)\hat{\psi}(r, t) \right\rangle \left\langle \hat{\psi}^\dagger(r', t)\hat{\psi}(r', t) \right\rangle}$$

(6.8)
and the approximations in [94] to obtain the expression

\[ g^{(2)}(r, r, t) = 2 - \frac{n_c(r, t)}{n_c(r, t) + \bar{n}(r, t)} \]  \hspace{1cm} (6.9)

for the second-order coherence function for the BEC. We approximate the second-order coherence of the output beam as prescribed in [94] by

\[ g^{(2)}(t) = 2 - \frac{\int dr V_c(r, t)n_c(r, t)}{\int dr V_c(r, t) (n_c(r, t) + \bar{n}(r, t))}. \] \hspace{1cm} (6.10)

We note that \( g^{(2)} = 1 \) indicates a second order coherent gas, whereas \( g^{(2)} = 2 \) would indicate total incoherence (a purely thermal gas). In this way we can quantify the coherence of the out-coupled beam.

### 6.3 Simulations for Adiabatic Evaporative Cooling Process

We consider here a dilute Bose gas consisting of 2000 \(^{87}\)Rb atoms in an axially symmetric harmonic trap, with radial and axial harmonic trapping frequencies of \( \omega_r = 2\pi \times 10\text{Hz} \) and \( \omega_z = 2\pi \times 400\text{Hz} \) respectively, having a transition temperature of \( T_c \lesssim 14\text{nK} \). Thus the axial confinement is sufficiently strong that all excited axial states may be neglected, hence the axial (z) component can be integrated out, and the BEC may effectively be treated as two-dimensional\(^1\). We perform time-dependent HFB calculations to simulate a cold dilute Bose gas initially at \( T = 12.5\text{nK} \), undergoing evaporative cooling. In all cases atoms are coupled out of the BEC using a complex coupling potential in the form of an annulus of radius \( a_c \) having a Gaussian cross-sectional profile with amplitude \( A_c \) and a full-width at half maximum (FWHM) of \( 2\sqrt{\ln 2} \) given by

\[ V_c(r, \theta, t) = A_c \exp \left[ -\left( \frac{r - a_{c_i} + (a_{c_i} - a_{c_f})t}{s_c} \right)^2 \right] \]  \hspace{1cm} (6.11)

during the time of cooling, i.e for \( 0 \leq t \leq T_{\text{cool}} \), with various amplitudes varying between \( 0.1\hbar\omega_r/2 \) and \( 200\hbar\omega_r/2 \) depending on the duration of cooling \( T_{\text{cool}} \), and with a FWHM of \( w_{\text{FWHM}} = 4.16r_0 \). The initial radius of the out-coupling potential is \( a_{c_i} = 8.5r_0 \) and is moved in to a final radius of \( a_{c_f} = 5.5r_0 \) at a constant rate determined by the time of cooling \( T_{\text{cool}} \). After the time of cooling, the outcoupling potential is switched off, i.e

\(^1\)Since \( T_{\text{max}} = 12.5\text{nK} \), the criteria for the two-dimensional approximation are satisfied - see section 5.2.2.
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$V_c(r, \theta, t) = 0$, for $t > T_{\text{cool}}$. At the initial radius of $8.5r_0$ the thermal and condensate densities, and hence the out-coupled beam are completely negligible. This should simulate an RF knife used in BEC cooling experiments. However, it should be pointed out that here we are cooling a BEC, whereas in an experiment a BEC is created by evaporative cooling of a thermal cloud above the condensation transition temperature. This is due to the limitations of the HFB formalism which is only valid in the presence of a condensate, and does not predict the growth of a condensate from a thermal cloud. Four cooling simulations were performed with cooling times of 15 trap cycles, 1 trap cycle, 0.1 trap cycles, and 0.01 trap cycles, thus the behaviour of the BEC can be determined for cooling periods varying by several orders of magnitude. Since the out-coupling potential always lies outside the Thomas-Fermi radius, more thermal particles than condensate particles are coupled out of the condensate, hence the BEC is effectively cooled during this process. This is reflected in the results shown in figure 6.1 which show the condensate and thermal fractions, and the $g^{(2)}$ correlation functions\(^2\) for each of the simulations, each of the cooling times differing by an order of magnitude. In all four cases, the condensate function increases substantially, resulting in a cooling of the BEC. At various points during the cooling process, an effective temperature is estimated by assuming that the process is quasi-static. Hence the time-independent HFB formalism can be used to determine the effective temperature for a given thermal density and total number of particles by an iterative process. The effective temperature is initially estimated using the ideal gas law for a 2D system where the condensate fraction $F_c$ is given by [107]

$$F_c = 1 - \left(\frac{T}{T^{2D}_c}\right)^2$$

(6.12)

where $T^{2D}_c$ is the predicted transition temperature for the ideal gas calculated according to the formula

$$k_B T^{2D}_c = \hbar \sqrt{6\omega_{\text{trap}} N^{1/2}} / \pi.$$  

(6.13)

(here $T^{2D}_c \approx 16.7 \text{nK}$). Thus the thermal fraction can be written as

$$\tilde{F} = \left(\frac{T}{T^{2D}_c}\right)^2.$$  

(6.14)

Let $\tilde{F}_i$ be the initial thermal fraction (i.e. prior to cooling) and $N_i$ the initial number of atoms, and $\tilde{F}$ the thermal fraction and $N$ the number of atoms at the time of the effective

---

\(^2\)We see from figures 6.1 I (c), II (c), and III (c) that the $g^{(2)}$ correlation of the out-coupled beam varies between $\sim 1.8$ at the start of the evaporative cooling, diminishing to $\sim 1.4$ at the end. This indicates a predominance of thermal atoms in the out-coupled beam, with the proportion of condensate atoms increasing as the out-coupling potential moves inwards. As pointed out earlier, the predominance is due to the fact that the out-coupling potential lies well outside the Thomas-Fermi radius, and this is reflected in the out-coupled beam being largely incoherent.
Figure 6.1: Cooling of BEC by in-moving annular out-coupling Gaussian potential for $r_{c_{\text{init}}} = 8.5r_0$, $r_{c_{\text{final}}} = 5.5r_0$, (I) over 15 trap cycles, (II) over 1 trap cycle, (III) over .1 trap cycles, and (IV) over .01 trap cycles, showing (a) change in condensate fraction, (b) change in thermal fraction, (c) $g^{(2)}$ correlation of out-coupled beam between times indicated by arrows on figures. Note that cooling only takes place between the times indicated by the arrows.
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Figure 6.2: (Colour on-line) Cooling of BEC by in-moving annular out-coupling Gaussian potential for $r_{c\text{init}} = 8.5r_0$, $r_{c\text{final}} = 5.5r_0$, (I) over 15 trap cycles, (II) over 1 trap cycle, (III) over .1 trap cycles, and (IV) over .01 trap cycles, showing (a) total number of atoms, (b) estimated effective temperature, and (c) deviation in condensate (solid black circles) and thermal densities (solid red diamonds). Note that cooling only takes place between the times indicated by the arrows.
Figure 6.3: (Colour on-line) Cooling of BEC by in-moving annular out-coupling Gaussian potential for $r_{c_{\text{ini}}} = 8.5r_0$, $r_{c_{\text{fin}}} = 5.5r_0$, showing condensate density (dashed black line) and fitted condensate density (solid black line) and (insert) thermal density (dashed red line) and fitted thermal density (solid red line) (I) for simulation 1 at times 0, 3, 7, 11, 15, and 19, and (II) for simulation 2 at times 0.25, 0.5, 0.75, 1, 2, and 5 trap cycles after out-coupling potential switched off. All densities are in units of $N r_0^{-2}$, and all distances in harmonic oscillator units $r_0$. 

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Figure 6.4: (Colour on-line) Cooling of BEC by in-moving annular out-coupling Gaussian potential for $r_{\text{cinit}} = 8.5r_0$, $r_{\text{cfinal}} = 5.5r_0$, showing condensate density (dashed black line) and fitted condensate density (solid black line) and (insert) thermal density (dashed red line) and fitted thermal density (solid red line) (I) for simulation 3 at times 0.025, 0.05, 0.1, 0.5, 1, 5 and 9, and (II) for simulation 4 at times 0.003, 0.007, 0.01, 0.1, 1, and 4 trap cycles after out-coupling potential switched off. All densities are in units of $N r_0^{-2}$, and all distances in harmonic oscillator units $r_0$. 
temperature estimate. Then the temperature may be estimated from equations (6.13) and (6.14) according to
\[ T_{\text{eff}} \approx \sqrt{\frac{\tilde{N}}{\tilde{N}_i}} T_i \]  
(6.15)
where \( \tilde{N} = N \tilde{F} \) is the number of thermal particles at the time of the calculation, and \( \tilde{N}_i = N_i \tilde{F}_i \) is the initial number of thermal particles in the BEC. The time-independent HFB equations (4.30) and (4.22) are then solved iteratively using this initial estimate for \( T_{\text{eff}} \), given the number of atoms remaining, such that the thermal fraction is the same as at that time in the cooling experiment. Thus one is able to establish an effective temperature at any point subject to the assumption of a quasi-static system. Figure 6.2 shows the estimated effective temperature for each of the simulations at various stages during the cooling process. Also shown in figure 6.2 are the number of atoms left, and the deviation between the time-dependent and the fitted time-independent condensate and thermal densities. Here we have defined the deviation \( \sigma \) between the time-dependent density \( n_{TD} \) at time \( t \), and the fitted time-independent density \( n_{\text{est}} \)
\[ \sigma(t) \equiv \sqrt{2} \sqrt{\frac{\sqrt{\int \text{d}r \left( n_{TD}(r, t) - n_{\text{est}}(r, t) \right)^2 \text{d}r}}{\int \text{d}r \left( n_{TD}(r, t) + n_{\text{est}}(r, t) \right)^2}}. \]  
(6.16)
Thus for the condensate the deviation \( \sigma_c \) would be defined for the densities \( n_{cTD} \) and \( n_{c\text{est}} \), and for the thermal population the deviation \( \sigma_t \) for the densities \( \tilde{n}_{TD} \) and \( \tilde{n}_{\text{est}} \). In simulations 1 and 2 the assumption of a quasi-static system is shown to be reasonable in that the cooling process is on a time-scale that allows for equilibration of the system. However, there is still a finite deviation due to numerical limitations imposed by the mode cut-off which drastically reduces the number of accessible states, the fact that we assume a time-independent quasi-particle basis at the initial temperature, with the initial quasi-particle spectrum, and the absence of higher order scattering processes in the HFB formalism, hence the differences in the profiles. We see from figure 6.3 that the forms of the density profiles are still similar, thus we can reasonably conclude that the assumption of a quasi-static process is justified in the first two simulations. Simulations 3 and 4, however, are no longer quasi-static processes since the time-scales of the cooling process do not allow for equilibration during the cooling process. This is indicated by a sharp increase in the deviations between the condensate and thermal densities shown in figure 6.2, and the qualitative differences in the thermal densities as seen in figure 6.4. From these calculations we can also establish the optimal way to achieve evaporative cooling of a BEC using an annular out-coupling potential as described above. We see from the above that it is desirable for the out-coupling to start from as far off-axis as possible - i.e. in regions where
there is negligible condensate density (i.e. annular radius $\gg$ Thomas-Fermi radius), and
to move this in sufficiently slowly so as to maximise the number of thermal atoms and
to minimise the number of condensate atoms coupled out of the BEC. We expect this
to be the case in view of the fact that most of the condensate atoms reside within the
Thomas Fermi radius, whereas we would expect a reasonable proportion of the thermal
atoms to lie outside the Thomas Fermi radius at temperatures $^3 T \gtrsim T_c/2$. Here we started
with a condensate at $T = 12.5\text{nK} \ (\sim 3T_c/4)$ with a thermal fraction of $\sim .25$. After the
adiabatic cooling, the thermal fraction was $\sim .1$, corresponding to an effective temperature
of $\sim 5\text{nK}$. This is confirmed in our result as shown in figures 6.1 and 6.2 where we see that
the maximum cooling is achieved in simulation 1 for the slowest rate of cooling. However,
simulation 2 is optimal in terms of efficiency of cooling when the time of cooling is also
taken into consideration, and is therefore preferable since this would minimise other losses
such as three-body losses which would become significant over the much longer cooling
times.

We note that there is no evidence of condensate growth in any of our simulations. Sim-
ulations at temperatures much closer to the transition temperature ($\sim 0.9T_c$), where the
condensate population is very small also show no evidence of condensate growth. This
is due to the fact that significant damping processes (probably the Landau and Beliaev
processes) are not accounted for in HFB due to the quadratic approximation of the Hamil-
tonian, which precludes the terms involving the Landau and Beliaev processes. Hence there
is no equilibration of the system within the time-scales of the experiment, and there is no
condensate growth, as one would have anticipated. Hence, whilst we do observe cooling of
the BEC, we don’t observe evaporative cooling leading to the growth of a condensate as
we would in an experiment.

$^3$Here $T_c$ is the transition temperature of the BEC, and is somewhat lower than the ideal gas predicted
transition temperature of $T_c^{2D} \approx 16.7\text{nK}$. We estimate that $T_c \lesssim 14\text{nK}$. 

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Chapter 7

Vortices in Quasi-Two Dimensional BECs

7.1 Introduction

Quantised vortices are perhaps the single most striking manifestation of superfluidity. Of particular interest here are the dynamics of vortices in Bose Einstein condensates (BECs). In 1999, Matthews et. al. [96] used an off-axis resonant laser in order to provide a rotating gradient in the AC Stark shift across the condensate. The definitive experiment was conducted by Madison et. al. [97] (see also [98]) towards the end of 1999, in which a focused laser beam was used to stir a BEC of \(^{87}\text{Rb}\) confined in a magnetic trap. Various methods have been used to create and detect vortices, see, for example, [42, 85, 99–102].

Much of the earlier theoretical work on the dynamics of vortices (see, for example, [36–38, 79]) assumed zero temperature, and neglected the effects of the non-condensate dynamics on the overall dynamics of the vortex. The Bogoliubov spectrum has a lowest-lying energy that is negative, the so-called anomalous mode [39, 40, 82]. The lowest-lying energy is zero in the frame rotating at this frequency, leading one to conclude that this is the precessional frequency of the vortex [39, 40, 82].

Solving the Hartree-Fock-Bogoliubov (HFB) equations for an on-axis vortex at finite temperature in the Popov approximation in a regime having sufficiently strong interactions yields a positive lowest lying energy mode, referred to as the lowest core localised state (LCLS) [2, 3]. This was then generalised to a lower bound for the LCLS energy for an off-axis vortex [86]. In both cases it is argued that the thermal cloud acts as an effective
potential, thereby stabilising the vortex, but this fails to take into account the dynamics of the thermal cloud itself. The association of this energy with the precessional frequency of the vortex [2,3] leads to the conclusion that the vortex precesses in the direction opposite to the condensate flow around the core. This is inconsistent with experiment and also seems intuitively unreasonable, since zero temperature predictions would suggest otherwise [39,40,82] and one might reasonably expect continuous variation with temperature. Later finite temperature calculations for off-axis vortices by Isoshima et. al. [4], however, conclude that no correlation exists between the precessional frequency and the anomalous mode.

To resolve this anomaly, we provide a full solution to the HFB equations for an off-axis vortex, making a novel use of the continuity equation for the condensate density to establish the vortex precessional frequency. Our model consists of a dilute Bose gas consisting of 2000 $^{87}$Rb atoms in an axially symmetric harmonic trap, with radial and axial harmonic trapping frequencies of $\omega_r = 2\pi \times 10$Hz and $\omega_z = 2\pi \times 400$Hz respectively, having a transition temperature of $T_c \lesssim 14$nK. Thus the axial confinement is sufficiently strong that all excited axial states may be neglected\(^1\), so the BEC may effectively be treated as two-dimensional, but not strong enough to affect the scattering, which is still essentially three-dimensional. Thus the BEC may be treated as two-dimensional from a computational viewpoint, since the axial dependency may be integrated out.

### 7.2 Time-Independent, Axially Symmetric Solutions

In view of the above argument, we restrict ourselves to two-dimensions, and use the dimensionless units in section (5.2.2). The 2D time-independent HFB equations in the dimensionless units used here are given by the GGPE (5.36) and the BdGEs (5.37).

Before commencing with our calculations for off-axis vortices and the predictions for their precessional frequencies, we perform time-independent on-axis vortex calculations in the Popov approximation as a comparison with the results of [2,3]. We make use of the axial symmetry of the condensate and quasi-particle wave-functions, obtaining a set of radial GGPEs and BdGEs for the case of a single on-axis vortex.

Let us consider a ground state having an on-axis vortex of vorticity $m$ ($m = 0$ corre-\(^1\) Here $T_{\max} = 7.5$nK, and therefore the criteria for the quasi-two-dimensional approximation are satisfied (see section 5.2.2).
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responds to a ground state having no vortices). The general expression for the condensate wavefunction expanded in the Laguerre basis is given by

\[ \Phi(r, \theta) = \sum_{l,n} a_{ln} \xi_{ln}(r, \theta) \]  

(7.1)

where the Laguerre basis function \( \xi_{ln}(r, \theta) \) is given by (see appendix C.1.5)

\[ \xi_{ln}(r, \theta) = e^{i l \theta} \sqrt{\frac{2}{\pi}} \xi_{ln}(r) \]  

(7.2)

with

\[ \xi_{ln}(r) = N_{n}^{l|} e^{-r^2/2} r^{|l|} L^{l|}_{n}(r^2) \]  

(7.3)

and where \( L^{l|}_{n}(r^2) \) is an associated Laguerre polynomial. The Laguerre basis function \( \xi_{ln}(r, \theta) \) satisfies the single-particle eigenvalue equation (as can be verified by substituting (C.26) into (5.35), and by applying (5.44))

\[ \hat{h}_{\Omega}(r, \theta) \xi_{ln}(r, \theta) = \left( \mu^{(SP)}_{ln} - l \Omega \right) \xi_{ln}(r, \theta) \]  

(7.4)

where we have defined (c.f. (5.35))

\[ \hat{h}_{\Omega}(r, \theta) = - \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right) + i \Omega \frac{\partial}{\partial \theta} + r^2, \]  

(7.5)

hence the motivation in using the Laguerre basis. In view of the axial symmetry of the solutions, we can write

\[ \Phi(r, \theta) = \frac{e^{im\theta}}{\sqrt{2\pi}} \Phi(r) \]  

(6.6)

where

\[ \Phi(r) = \sum_{n} a_{n} \xi_{mn}(r) \]  

(7.7)

where \( m \) is the vorticity of the on-axis vortex. Here the \( \{a_{ln}, l \neq m\} \) are considered to be zero since we are considering a vortex of vorticity \( m \), and we use the short-hand notation \( a_{n} \equiv a_{mn} \). Clearly the condensate density \( n_{c}(r, \theta) \) can be written as

\[ n_{c}(r, \theta) = \frac{1}{2\pi} n_{c}(r) \]  

(7.8)

We can also write the quasiparticle amplitudes \( u_{q}(r, \theta) \) and \( v_{q}(r, \theta) \) in the form

\[ u_{lq}(r, \theta) = \frac{e^{i(l+m)\theta}}{\sqrt{2\pi}} u_{lq}(r) \]  

(7.9)

\[ v_{lq}(r, \theta) = \frac{e^{i(l-m)\theta}}{\sqrt{2\pi}} v_{lq}(r) \]  

(7.10)
where
\begin{align}
u_{lq}(r) & = \sum_n c_{q,n} \xi_{l+m,n}(r) \\
v_{lq}(r) & = \sum_n d_{q,n} \xi_{l-m,n}(r).
\end{align}

(7.11)

Hence the thermal and anomalous densities \( \tilde{n}(r, \theta) \) and \( \tilde{m}(r, \theta) \) can be written as
\begin{align}
\tilde{n}(r, \theta) & = \frac{1}{2\pi} \tilde{n}(r) \\
\tilde{m}(r, \theta) & = \frac{e^{2im\theta}}{2\pi} \tilde{m}(r)
\end{align}

(7.12) and (7.13)

respectively. So, multiplying by \( e^{-im\theta}/\sqrt{2\pi} \) for the GGPE (5.36), and by \( e^{-i(l+m)\theta}/\sqrt{2\pi} \) and \( e^{-i(l-m)\theta}/\sqrt{2\pi} \) for the first and second of the BdGEs (5.37), and integrating over all \( \theta \), we obtain the time-independent radial HFB equations, where the radial time-independent GGPE is given by (5.47) (note the radial wave-function is real, i.e. \( \Phi^*(r) = \Phi(r) \))
\begin{align}
\Delta \mu \Phi(r) & = \left( \hat{h}_m(r) - \mu + C_{2D}^R \left( |\Phi(r)|^2 + 2\tilde{n}(r) \right) \right) \Phi(r) + C_{2D}^R \tilde{m}(r) \Phi(r) - \int_0^\infty r' dr' \hat{P}(r', r) \phi(r') \\
\end{align}

(7.14) and the radial BdGEs by (5.48)
\begin{align}
\epsilon_{lq} \begin{bmatrix} u_{lq}(r) \\ v_{lq}(r) \end{bmatrix} & = \int_0^\infty r' dr' \begin{bmatrix} Q_l(r, r') \hat{L}_{l+m}(r') & Q_l(r, r') \mathcal{M}(r') \\ -Q_l(r, r') \mathcal{M}(r') & -Q_l(r, r') \hat{L}_{l-m}(r') \end{bmatrix} \begin{bmatrix} u_{lq}(r') \\ v_{lq}(r') \end{bmatrix}
\end{align}

(7.15)

Here we have defined the radial operators \( \hat{L}_l(r) \) and \( \mathcal{M}(r) \) by (5.49)
\begin{align}
\hat{L}_l(r) & \equiv \hat{h}_l(r) - \mu + 2C_{2D}^R \left( |\Phi(r)|^2 + \tilde{n}(r) \right) \\
\mathcal{M}(r) & \equiv C_{2D}^R \left( \Phi^2(r) + \tilde{m}(r) \right)
\end{align}

(7.16)

and the operator \( \hat{P}(r', r) \) by (5.50)
\begin{align}
\hat{P}(r', r) & \equiv \left( \tilde{n}(r', r) \hat{L}(r') + \tilde{m}(r', r) \mathcal{M}(r') \right) / \sqrt{N_c(t)}
\end{align}

(7.17)

with \( \hat{h}_l(r) \) given by (5.51)
\begin{align}
\hat{h}_l(r) & \equiv - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{l^2}{r^2} - \mu + r^2.
\end{align}

(7.18)

The radial projection operator \( Q_l(r, r') \) is given by (5.53)
\begin{align}
Q_l(r, r') & = \delta(r - r') - \delta_{l,0} \phi(r) \phi(r')
\end{align}

(7.19)

The radial 2D nonlinearity constant \( C_{2D}^R \equiv C_{2D}/2\pi \) is given by (5.54)
\begin{align}
C_{2D}^R & = 4 \left( \frac{\lambda}{2\pi} \right)^{1/2} \frac{a_s}{r_0} N.
\end{align}

(7.20)
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Figure 7.1: On-axis time-independent solutions for standard HFB in the Popov approximation, (a) condensate density, (b) thermal density at $T = 1 \text{nK}$ (solid line) and $T = 5 \text{nK}$ (dashed line), (c) LCLS energy versus temperature, and (d) excitation energy spectrum vs angular quantum number $l$ - energies shown increasing with quantum number $n = 0, 1, \ldots$. All distances are in harmonic oscillator units $r_0$, densities in units $N r_0^{-2}$ where $N$ is the number of atoms, and energies in trap units $\hbar \omega_r$.

In the rotating frame $\hat{h}_{l,\Omega}(r)$ is given by (5.52)

$$
\hat{h}_{l,\Omega}(r) \equiv - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{l^2}{r^2} - l\Omega - \mu + r^2.
$$

(7.21)

Results comparable to those of [2,3] are reproduced by time-independent on-axis calculations in the Popov approximation. Similar calculations were done using orthogonal HFB. Figures 7.1(a),(b) and 7.2(a),(b) show the condensate and non-condensate density profiles in the plane passing through the vortex for the Popov and orthogonal HFB cases. Note that the thermal density for HFB is considerably less than for Popov. This is due to the upward shift in the low-lying excitation energies, which is clearly demonstrated in figures 7.1(c) and 7.2(c) which are plots of the LCLS energy versus temperature for the Popov and orthogonal HFB cases respectively. Here we see that the Popov LCLS values are substantially smaller than those for the orthogonal HFB case, and at $T = 0 \text{nK}$ we see that $\epsilon_{LCLS}$ for the orthogonal HFB case is not zero, but some very small positive energy. This is due to the energy gap problem associated with HFB. The full energy spectra for the Popov and orthogonal HFB cases are shown respectively in figures 7.1(d) and 7.2(d) as a function of the angular momentum quantum number $l$ for increasing quantum number $n = 0, 1, \ldots$. 

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Figure 7.2: On-axis time-independent solutions for orthogonal HFB, (a) condensate density, (b) thermal density at $T = 2\text{nK}$ (solid line) and $T = 7.5\text{nK}$ (dashed line), (c) LCLS energy versus temperature, and (d) excitation energy spectrum vs angular quantum number $l$ - energies shown increasing with quantum number $n = 0, 1, \ldots$. All distances are in harmonic oscillator units $r_0$, densities in units $N r^{-2}_0$ where $N$ is the number of atoms, and energies in trap units $\hbar \omega_r$.

7.3 Non-Axially Symmetric Solutions

Here we consider non-axially symmetric, time-independent solutions to the two-dimensional HFB equations (5.36) and (5.37). This would be the case where the ground state contains off-axis vortices. We shall solve such problems in the rotating frame (where stationary solutions may be found), where the precessional frequency of the vortex is predicted by (4.65) derived from the continuity equation for the condensate density in the rotating frame.

As mentioned in the previous section, the general solution for the condensate wave function is given in terms of the Laguerre basis functions $\{\xi_{ln}(r, \theta)\}$ (equations (7.2) and (7.3)) by (7.1)

$$\Phi(r, \theta) = \sum_{l, n} a_{ln} \xi_{ln}(r, \theta)$$

(7.22)

The quasiparticle amplitudes may likewise be expanded in terms of the Laguerre basis by

$$u_q(r, \theta) = \sum_{l, n} c_{q,ln} \xi_{ln}(r, \theta)$$

$$v_q(r, \theta) = \sum_{l, n} d_{q,ln} \xi_{ln}(r, \theta).$$

(7.23)

Before solving this problem for off-axis vortices, it is instructive to examine how vortices...
can be constructed in non-interacting or extremely weakly-interacting systems using a two-state model. We shall see that the predictions for the precessional frequencies are good for non-interacting or very weakly interacting systems, but are rather poor for even modestly interacting systems. We shall generalise this to a multi-state model, but will not solve this problem directly. Rather we shall use the continuity equation for the condensate density to predict the precessional frequencies, using modified basis functions to fix the position of the vortices, and show that the multistate model and the modified basis function method are equivalent and agree in their prediction of precessional frequencies in the limit of infinite energy cutoff.

7.3.1 Two-state Model in HFB

Let us consider two-mode superposition states of the form [90, 105]

\[ \Phi(r, \theta, t) = \frac{1}{\sqrt{2\pi}} \left( a_g(t)\phi_g(r) + a_v(t)\phi_v(r)e^{i\theta} \right) \]  

(7.24)

where

\[ a_g(t) = a_{g0}e^{-i\mu_g t} \]
\[ a_v(t) = a_{v0}e^{-i\mu_v t}. \]  

(7.25)

This is motivated by Rokshar’s work [79] where the many-body vortex ground state may be described by the superposition of the vortex condensate state and the core state (3.1)

\[ \Phi = \sqrt{1 - x_{\text{core}}} \Phi_m + e^{i\chi} \sqrt{x_{\text{core}}} \Phi_{\text{core}}. \]  

(7.26)

Here we identify

\[ \Phi_m \equiv \phi_g(r)/\sqrt{2\pi}, \quad \Phi_{\text{core}} \equiv \phi_v(r)/\sqrt{2\pi}, \quad \sqrt{1 - x_{\text{core}}} \equiv a_g \quad \text{and} \quad \sqrt{x_{\text{core}}} \equiv a_v. \]  

(7.27)

We thus identify \( \phi_v \) and \( \phi_g \) with the vortex and core (ground) states respectively, hence the subscripts \( v \) and \( g \) used in the notation in (7.24). Since there is Rabi oscillation between the two states, the vortex precesses at a frequency determined by the Rabi frequency. We solve this by transforming to the rotating frame. In the rotating frame

\[ \hat{h}(r, \theta) \to \hat{h}_{\Omega}(r, \theta) = \hat{h}(r, \theta) + i\Omega \frac{\partial}{\partial \theta} \]  

(7.28)

so

\[ \hat{h}(r) \to \hat{h}_{\Omega,t}(r) = \hat{h}(r) - \Omega \]  

(7.29)
In the co-rotating frame $\theta \rightarrow \theta - \Omega t$, a stationary solution can be found, and the ansatz (7.24) becomes
\[
\Phi(r, \theta, t) = e^{-i\mu t} \Phi(r, \theta) = e^{-i\mu t} \left( a_{g0} \phi_g(r) + a_{v0} \phi_v(r) e^{i\theta} \right)
\]
(7.30)
The chemical potential is given by
\[
\mu = \mu_g
\]
(7.31)
and the precessional frequency of the vortex by
\[
\Omega = \mu_v - \mu_g.
\]
(7.32)
Here we calculate the precessional frequency as predicted by the two-state model for various interaction strengths $C_{2D}^{R'} = \alpha C_{2D}^R$ where we use the parameter $\alpha \in [0, 1]$ to vary the interaction strength between 0 and $C_{2D}^R$.

**The Coupled GGPEs in the Rotating Frame**

In the frame rotating at the precessional frequency $\Omega$, we obtain the coupled GGPEs (see Appendix E.1.1)
\[
\mu \phi_g = \left[ \hat{h}_{\Omega,0} + C_{2D}^{R'} \left( n_{g0} |\phi_g|^2 + 2n_{v0} |\phi_v|^2 + 2\tilde{N}^{(0)} + \tilde{M}^{(0)} \right) \right] \phi_g + \frac{a_{v0}}{a_{g0}} C_{2D}^{R'} \left( 2\tilde{N}^{(1)} + \tilde{M}^{(-1)} \right) \phi_v
\]
(7.33)
and
\[
\mu \phi_v = \left[ \hat{h}_{\Omega,1} + C_{2D}^{R'} \left( n_{v0} |\phi_v|^2 + 2n_{g0} |\phi_g|^2 + 2\tilde{N}^{(0)} + \tilde{M}^{(-2)} \right) \right] \phi_v + \frac{a_{g0}}{a_{v0}} C_{2D}^{R'} \left( 2\tilde{N}^{(-1)} + \tilde{M}^{(-1)} \right) \phi_g
\]
(7.34)
where
\[
n_{g0} = |a_{g0}|^2,
\]
\[
n_{v0} = |a_{v0}|^2
\]
(7.35)
and where we have defined the quantities
\[
N^{(l)}(r) \equiv \int_0^{2\pi} \frac{e^{il\theta}}{\sqrt{2\pi}} n_c(r, \theta) d\theta,
\]
(7.36)
\[
\tilde{N}^{(l)}(r) \equiv \int_0^{2\pi} \frac{e^{il\theta}}{\sqrt{2\pi}} \tilde{n}(r, \theta) d\theta
\]
(7.37)
and
\[
\tilde{M}^{(l)}(r) \equiv \int_0^{2\pi} \frac{e^{il\theta}}{\sqrt{2\pi}} \tilde{m}(r, \theta) d\theta.
\]
(7.38)
Then if we define the operators $\hat{F}_{g,\Omega}$, $G_g$, $\hat{F}_{v,\Omega}$, and $G_v$ for the rotating frame rotating about the axis of symmetry at angular frequency $\Omega$ given respectively by

$$\hat{F}_{g,\Omega} \equiv \hat{h} \Omega, 0 + C_{2D}^{R} \left(n_{g0} |\phi_g|^2 + 2n_{v0} |\phi_v|^2 + 2\tilde{N}^{(0)} + \tilde{M}^{(0)}\right) = \hat{F}_g$$  (7.39)

$$G_g \equiv \frac{a_{v0}}{a_{g0}} C_{2D}^{R} \left(2\tilde{N}^{(1)} + \tilde{M}^{(-1)}\right)$$  (7.40)

$$\hat{F}_{v,\Omega} \equiv \hat{h} \Omega, 1 + C_{2D}^{R} \left(n_{v0} |\phi_v|^2 + 2n_{g0} |\phi_g|^2 + 2\tilde{N}^{(0)} + \tilde{M}^{(-2)}\right) = \hat{F}_v - \Omega$$  (7.41)

and

$$G_v \equiv \frac{a_{g0}}{a_{v0}} C_{2D}^{R} \left(2\tilde{N}^{(-1)} + \tilde{M}^{(-1)}\right),$$  (7.42)

the GGPEs in the rotating frame can be rewritten in the matrix form

$$\mu \begin{bmatrix} \phi_g \\ \phi_v \end{bmatrix} = \begin{bmatrix} \hat{F}_{g,\Omega} & G_g \\ G_v & \hat{F}_{v,\Omega} \end{bmatrix} \begin{bmatrix} \phi_g \\ \phi_v \end{bmatrix},$$  (7.43)

The BdGEs

We note that we can write

$$u_q(r, \theta) = \sum_{nl} c_{q,ln} \xi_{ln}(r) e^{il\theta} / \sqrt{2\pi} = \sum_l u_q^{(l)}(r) e^{il\theta} / \sqrt{2\pi}$$

$$v_q(r, \theta) = \sum_{nl} d_{q,ln} \xi_{ln}(r) e^{il\theta} / \sqrt{2\pi} = \sum_l v_q^{(l)}(r) e^{il\theta} / \sqrt{2\pi}.$$  (7.44)

Let us define the quantities $\hat{L}_u^{(u)}$, $\hat{L}_v^{(v)}$, $\hat{M}_u^{(u)}$, and $\hat{M}_v^{(v)}$ as in appendix E.1.2. Then it can be shown for the quasiparticle amplitudes in the rotating frame that (see appendix E.1.2)

$$\epsilon_q u_q^{(l)} = \sum_{l'} \left(\hat{L}_u^{(u)} u_q^{(l')} + \hat{M}_u^{(u)} v_q^{(l')}\right)$$  (7.45)

and

$$-\epsilon_q v_q^{(l)} = \sum_{l'} \left(\hat{L}_v^{(v)} v_q^{(l')} + \hat{M}_v^{(v)} u_q^{(l')}\right)$$  (7.46)

This can be rewritten in the matrix form

$$\begin{bmatrix} \hat{L}_u & \hat{M}_u \\ -\hat{M}_v & -\hat{L}_v \end{bmatrix} \begin{bmatrix} u_q \\ v_q \end{bmatrix} = \epsilon_q \begin{bmatrix} u_q \\ v_q \end{bmatrix},$$  (7.47)

where we have defined the vectors $\mathbf{u}_q$ and $\mathbf{v}_q$, and the matrix operators $\hat{L}_u$, $\hat{L}_v$, $\hat{M}_u$, and $\hat{M}_v$ as in appendix E.1.2. We solve the two-state GGPE (7.43) and BdGEs (7.47) for values of $\alpha$ lying between 0 and 1 and for various values of $a_g$ and $a_v$ in the zero temperature limit.

A vortex detection algorithm is used to determine the distance $a$ of the vortex from the axis for each combination $a_a$, $a_v$ for the different interaction strength parameters $\alpha$. We
use cubic spline interpolation to determine the relationship of the precessional frequency Ω as a function of the distance $a$ of the vortex from the axis, and of the interaction strength parameter $\alpha$. Hence one is able to plot the precessional frequency of the vortex $\Omega$ versus $a$ for various values of the interaction strength parameter $\alpha$, and also the precessional frequency $\Omega$ versus interaction strength parameter $\alpha$ at various distances $a$ of the vortex from the axis. One can also use cubic spline interpolation to extrapolate the plot of $\Omega$ versus $a$ to $a = 0$, and hence we can plot the extrapolated on-axis precessional frequency $\Omega_{\text{extrap}}$ versus $\alpha$ and compare these with the anomalous mode frequencies calculated using the Bogoliubov spectrum [39, 40, 82]. Figure 7.3(a) shows a plot of the two state on-axis extrapolated results $\Omega_{\text{extrap}}$ versus $\alpha$ compared with the predictions by the anomalous mode frequencies $\Omega_{\text{anom}}$ versus $\alpha$, and reveals that agreement is reasonable only for small values of $\alpha$. This is understandable in view of the increasing non-linearity. As expected, the superposition approximation is only valid for small $\alpha$, hence the rapid departure in agreement as $\alpha$ increases. For $\alpha \gtrsim 0.1$, the results cease to be meaningful. Figure 7.3(b) shows a plot of the two-state precessional frequency $\Omega$ versus vortex position $a$ for various values of the interaction strength parameter $\alpha$. Later we will see that the precessional frequencies predicted using the continuity equation for the condensate density agree well.
with the anomalous mode frequencies in the on-axis, $T = 0$ limit, in contrast with the two-state model prediction here.

### 7.3.2 Generalised Multi-state Model in HFB

We generalise the two-state model [90, 105], and write the following ansatz for the condensate wave function

$$
\Phi(r, \theta, t) = e^{-i\mu t} \frac{1}{\sqrt{2\pi}} \left( a_g \sum_{l \neq 1} e^{-i\Omega t} \phi_g^{(l)}(r)e^{il\theta} + a_v e^{-i\Omega t} \phi_v(r)e^{i\theta} \right) \tag{7.48}
$$

This also has the general form (3.1) of Rokshar’s superposition state [79]

$$
\Phi = \sqrt{1 - x_{\text{core}}} \Phi_m + e^{ix} \sqrt{x_{\text{core}}} \Phi_{\text{core}}.
$$

Here we identify

$$
\Phi_m \equiv \sum_{l \neq 1} e^{-i(\theta - \Omega t)} \phi_g^{(l)}(r)/\sqrt{2\pi}, \quad \Phi_{\text{core}} \equiv \phi_v(r)/\sqrt{2\pi}, \quad \sqrt{1 - x_{\text{core}}} \equiv a_g, \quad \sqrt{x_{\text{core}}} \equiv a_v.
$$

In the co-rotating frame $\theta \to \theta - \Omega t$, a stationary solution can be found in the rotating frame. We have, as before (7.28), (7.29)

$$
\hat{h}(r, \theta) \to \hat{h}_{\Omega}(r, \theta) = \hat{h}(r, \theta) + i\Omega \frac{\partial}{\partial \theta}
$$

so

$$
\hat{h}_l(r) \to \hat{h}_{\Omega,l}(r) = \hat{h}_l(r) - \Omega l.
$$

### The Coupled GGPEs

In the co-rotating frame $\theta \to \theta - \Omega t$ the ansatz (7.48) becomes (after cancellation of phase factors)

$$
\Phi(r, \theta, t) = e^{-i\mu t} \Phi(r, \theta) = e^{-i\mu t} \frac{1}{\sqrt{2\pi}} \left( a_g \sum_{l \neq 1} \phi_g^{(l)}(r)e^{il\theta} + a_v \phi_v(r)e^{i\theta} \right) \tag{7.49}
$$

so in the rotating frame we have the time-independent GGPE, where we have neglected the orthogonality projection part of (7.14).

$$
\mu \Phi = \left[ \hat{h}_{\Omega} + C^{R}_{2D} \left(n_c + 2\tilde{n} \right) \right] \Phi + C^{R}_{2D} \tilde{m} \Phi^* \tag{7.50}
$$

Note that the wave-function $\Phi(r, \theta)$ can no longer be assumed to be real, as we did in section 7.2. We now have an off-axis vortex which implies that $\Phi(r, \theta)$ must be complex.
Substituting the ansatz (7.49) into the above, multiplying by \( e^{-il\theta}/\sqrt{2\pi} \) for \( l = 0, \pm 1, \ldots \) and integrating over all \( \theta \), we obtain the coupled GGPEs

\[
\mu \phi^{(l)}(r) = \left[ \hat{h}_l - \Omega l \right] \phi^{(l)}(r) + C_{2D}^R \sum_{l' \neq 1} \left( N_l^{(l')-} + 2\tilde{N}^{(l')-} + \tilde{M}^{(l')-} \right) \phi^{(l')}(r) + \frac{2\tilde{a}_g C_{2D}^R}{a_g} \sum_{l' \neq 1} \left( N_l^{(1-l) -} + 2\tilde{N}^{(1-l) -} + \tilde{M}^{(1-l) -} \right) \phi^{(l')}(r) \tag{7.51}
\]

for \( \phi^{(l)}_g \), and

\[
\mu \phi_v(r) = \left[ \hat{h}_1 - \Omega + C_{2D}^R \left( N_0^{(0)} + 2\tilde{N}^{(0)} + \tilde{M}^{(-2)} \right) \right] \phi_v(r) + \frac{2\tilde{a}_g C_{2D}^R}{a_g} \sum_{l' \neq 1} \left( N_l^{(l')-} + 2\tilde{N}^{(l')-} + \tilde{M}^{(l')-} \right) \phi^{(l')}(r) \tag{7.52}
\]

for \( \phi_v(r) \).

### 7.3.3 Constraint equations for \( \mu \) and \( \Omega \)

We first note the normalisation conditions

\[
\sum_{l \neq 1} \int_{-\infty}^{\infty} r dr \phi^{(l)}_g^2(r) = 1 \tag{7.53}
\]

and

\[
\int_{-\infty}^{\infty} r dr \phi_v^2(r) = 1. \tag{7.54}
\]

Since the factors \( a_g \), and \( a_v \) also satisfy the normalisation condition

\[
|a_g|^2 + |a_v|^2 = 1 \tag{7.55}
\]

the normalisation condition

\[
\int_0^{2\pi} \int_0^{\infty} r dr d\theta |\Phi(r, \theta)|^2 = \int_0^{\infty} r dr N_0^{(0)}(r) = 1 \tag{7.56}
\]

is satisfied, as required.

We expand \( \phi^{(l)}_g(r) \) and \( \phi_v(r) \) in the single particle basis \( \{ \xi_n(r) \} \) as in (E.45) and (E.46) and substitute into the GGPE (7.51) for the core state and the GGPE (7.52) for the vortex state. It can be shown using the above normalisation conditions (see derivation in appendix E.2.2) that

\[
\mu = K_v - \frac{K_g - K_v}{C_g - 1} \tag{7.57}
\]

and

\[
\Omega = \frac{K_g - K_v}{C_g - 1}. \tag{7.58}
\]
where the quantities $C_g$, $K_g$ and $K_v$ are given respectively by the expressions (E.63), (E.64) and (E.65). In the next section we will compare the precessional frequencies as calculated by equation (7.58) with those predicted using the continuity equation for the condensate density.

### 7.4 Creation of Off-axis Vortices

#### 7.4.1 Single Vortex

We find stationary solutions for a single off-axis vortex by solving the 2D HFB equations (5.36) and (5.37) and the equation for the precessional frequency (4.65) in the frame rotating at the predicted precessional frequency, where $A(r, \theta)$ and $B(r, \theta)$ are given by (4.62) and (4.63) with $C(r, \theta)$ and $G(r, \theta)$ calculated for orthogonal HFB according to (4.125) and (4.126) respectively, i.e.

$$
\Omega = \frac{\int_0^{2\pi} \int_0^\infty A(r, \theta)B(r, \theta)rdrd\theta}{\int_0^{2\pi} \int_0^\infty r^2 (A(r, \theta))^2 rdrd\theta}
$$

where

$$A(r, \theta) \equiv \left( R \frac{\partial R}{\partial \theta} + I \frac{\partial I}{\partial \theta} \right)$$

and

$$B(r, \theta) \equiv \frac{\hbar}{2m} \left[ r^2 \left( R \frac{\partial^2 I}{\partial r^2} - I \frac{\partial^2 R}{\partial r^2} \right) + r \left( R \frac{\partial I}{\partial r} - I \frac{\partial R}{\partial r} \right) + \left( R \frac{\partial^2 I}{\partial \theta^2} - I \frac{\partial^2 R}{\partial \theta^2} \right) \right] + \frac{r^2}{2\hbar} C(r, \theta)
$$

with $C(r, \theta)$ and $G(r, \theta)$ given by

$$
C(r, \theta) \equiv g \left( \bar{m}(r, \theta)\Phi^* (r, \theta) \Phi^2 (r, \theta) - \bar{m}^*(r, \theta)\Phi^2 (r, \theta) \right) + G^*(r, \theta) - G(r, \theta)
$$

$$
G(r, \theta) \equiv \Phi^* (r, \theta) \int_0^{2\pi} \int_0^\infty rdr'd\theta' \hat{P}(r', \theta', r, \theta)\phi(r', \theta')
$$

Here the quantities $R(r, \theta)$ and $I(r, \theta)$ are the real and imaginary parts of the condensate wave-function $\Phi(r, \theta)$ as defined in (4.59), section 4.2.7. The effect of the projection operator $\hat{P}(r', \theta', r, \theta)$ is small, and implies an unnecessary increase in the computation required in solving the orthogonal time-independent HFB equations. Calculations using the full orthogonal formalism reveal that $\hat{P}(r', \theta', r, \theta)$ can be neglected in the time-independent case\(^2\). This operator is critically important, however, in time-dependent calculations using the orthogonal time-dependent orthogonal HFB equations, as neglect of this term leads

\(^2\)See calculations in appendix F.3.
to violation of angular momentum conservation. The effect on time-independent calculations is, however, negligible, and we will neglect all terms involving \( \hat{P}(r', \theta', r, \theta) \) in all our time-independent calculations. In this case the expression \( C(r, \theta) \) simplifies to

\[
C(r, \theta) \equiv g \left( \tilde{m}(r, \theta)\Phi^*(r, \theta) - \tilde{m}^*(r, \theta)\Phi^2(r, \theta) \right)
\]

(7.63)
as for standard HFB. Suppose we have a single vortex situated at position \((r_1, \theta_1)\). Then we can write the condensate wave function \( \Phi(r, \theta) \) in terms of the modified basis functions \( \{ \chi_{ln}^{(1)}(r, \theta) \} \) given by (5.65)

\[
\chi_{ln}^{(1)}(r, \theta) \equiv \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_1, \theta_1)}{\xi_{10}(r_1, \theta_1)}\xi_{10}(r, \theta)
\]

(7.64)
as defined in section 5.3.1 in chapter 5. This gives the necessary constraint for the vortex to be at this position. Here the \( \{ \xi_{ln}(r, \theta) \} \) are the Laguerre basis functions given by

\[
\xi_{ln}(r, \theta) = \frac{e^{il\theta}}{\sqrt{2\pi}} \left( \frac{2n!}{(n+|l|)!} \right)^{1/2} e^{-r^2/2} r^{|l|} L_n^{|l|}(r^2)
\]

(7.65)
and where \( L_n^{|l|}(x) \) is a modified Laguerre polynomial of order \( n \). Thus we can write the condensate wave-function as

\[
\Phi(r, \theta) = \sum_{l,n \in S^{(1)}} a_{ln} \chi_{ln}^{(1)}(r, \theta).
\]

(7.66)
where we have defined

\[
S^{(1)} \equiv \{ l, n | (l, n) \in S - \{ (1, 0) \} \}
\]

(7.67)
with \( S \equiv \{ l, n | n = 0, \ldots, l = 0, \pm 1, \ldots \} \). This procedure is valid provided the vortex position \((r_1, \theta_1)\) does not lie on any of the roots of the Laguerre basis functions \( \{ \xi_{ln}(r, \theta) \} \).

### 7.4.2 Multiple Vortices

This procedure may be extended to \( N_v \) vortices by writing the condensate wave function \( \Phi(r, \theta) \) in terms of the modified basis functions \( \{ \chi_{ln}^{(N_v)}(r, \theta) \} \)

\[
\Phi(r, \theta) = \sum_{l,n \in S^{(N_v)}} a_{ln} \chi_{ln}^{(N_v)}(r, \theta)
\]

(7.68)
where the modified basis functions \( \{ \chi_{ln}^{(N_v)}(r, \theta) \} \) for \( N_v \) vortices situated at positions \((r, \theta) \in \{(r_i, \theta_i) | i = 1, \ldots N_v \} \) are defined by (5.70)

\[
\chi_{ln}^{(N_v)}(r, \theta) \equiv \chi_{ln}^{(N_v-1)}(r, \theta) - \frac{\chi_{ln}^{(N_v-1)}(r_{N_v}, \theta_{N_v})}{\chi_{N_v,0}^{(N_v-1)}(r_{N_v}, \theta_{N_v})} \chi_{N_v,0}^{(N_v-1)}(r, \theta)
\]

(7.69)
in section (5.3.1) in chapter 5, where we have generalised the definition (7.67) in the single vortex case to

$$\mathcal{S}^{(N_v)} \equiv \{l, n \mid (l, n) \in \mathcal{S} - \{(1, 0), \ldots, (N_v, 0)\}\} \quad (7.70)$$

in the multi-vortex case.

### 7.4.3 Finite Temperature Time-independent Calculations for Off-axis Vortices

Stationary solutions are found in the rotating frame for the single vortex case, and also in the case of multiple vortices, provided the interactions between the vortices are not too strong. In cases where there are strong interactions between vortices, approximately stationary solutions can be found, establishing lower and upper bounds for the precessional frequency, and the precessional frequency determined more accurately in time-dependent simulations.

Figures 7.4(a) and (b) show the condensate and non-condensate density profiles in the plane passing through the vortex for the Popov and HFB cases for a vortex situated at $a = 0.5$ radial harmonic oscillator units from the axis, at temperature $T_c = 5\text{nK}$. Note in particular that the thermal density for HFB is considerably less than for Popov. As in the on-axis case, this is due to the upward shift in the lower-lying excitation energies.

One would expect the precessional frequency $\Omega$ to vary smoothly with temperature $T$, and the time-independent off-axis calculations for a variety of different vortex positions for the Popov and the HFB cases reveal that this is indeed the case, and also reveal consistency with off-axis GPE calculations, which coincide almost exactly with the HFB $T = 0$ calculations (see figures 7.5(a) and (b)). Figures 7.5 (a),(b) and (c),(d) shows respectively the precessional frequency and the LCLS energy plotted as a function of vortex position $a$ at temperatures 0nK, 2nK, 5nK and 7.5nK or as a function of temperature $T$ at vortex positions 0.1, 0.5, 0.8 and 1.1 harmonic oscillator units.

One would also expect the precessional frequency $\Omega$ to vary smoothly with $a$, so to check the consistency of the on-axis and off-axis calculations, one needs to determine $\Omega$ for the on-axis case by extrapolation, thus one expects $\Omega_{\text{on-axis}} \approx \Omega_{\text{extrap}}$. Solving for the on-axis case in the frame rotating at the extrapolated precessional frequency $\Omega_{\text{extrap}}$ for both the Popov approximation and the full HFB, one finds consistency in the precessional frequencies.
Figure 7.4: (a) (Colour on-line) HFB Popov Condensate fraction (black solid line) and thermal density (red dashed line) versus position in trap in plane passing through vortex, (b) HFB condensate fraction (black solid line) and thermal density (red dashed line) versus position in trap in plane passing through vortex, and (c) and condensate fraction $N_c$ versus $T$ for ideal gas (dashed line), HFB at position 0.5 (black dots) and off-axis Popov calculations for condensate rotating at extrapolated precessional frequency for mode cutoff of 100 modes (red triangles), and 1639 modes (red squares). All distances are in harmonic oscillator units $r_0$, and densities in units $N r_0^{-2}$ where $N$ is the number of atoms.

and the LCLS energies as shown for the HFB case\(^3\) in figure 7.7 where $\epsilon_{\text{LCLS}_{\text{on-axis}}}$ at $\Omega_{\text{extrap}}$ and $\epsilon_{\text{LCLS}_{\text{extrap}}}$ are plotted as a function of temperature and the LCLS energies for the off-axis calculations plotted in figures 7.5(c),(d) as a function of vortex position $a$ and temperature $T$ respectively. These energies also correspond to the LCLS energies calculated perturbatively in [106]. Here they make use of first order perturbation theory to calculate the LCLS energy for a disk-shaped condensate of size given by the Thomas-Fermi radii with a singly-quantised vortex in an axi-symmetric trap, rotating with frequency $\Omega$. Neglecting the vortex curvature, they obtain the result

$$
\epsilon_{\text{LCLS}} = \frac{\epsilon_a}{2} \left( \sqrt{ \left( 1 - \frac{\hbar \Omega}{\epsilon_a} \right)^2 + \frac{4 \gamma k_B T}{\epsilon_a} } - \left( 1 - \frac{\hbar \Omega}{\epsilon_a} \right) \right)
$$

(7.71)

where $\epsilon_a = (3\hbar^2 \omega_r / 4\mu) \ln (R_r / \xi)$ and $\gamma = 0.077 R_r^2 / N \xi^4$, and where $\xi$ is the healing length of the condensate with $R_r$ the Thomas-Fermi radius for a trap rotating at frequency $\Omega$. Reference to figure 7.8 shows good agreement of the LCLS energies predicted by the orthogonal HFB in the LAB frame (see also figure 7.2(c)) with the LCLS energies calculated using (7.71) for $\Omega = 0$ (LAB frame). We note a small but finite positive value for the $\epsilon_{\text{LCLS}}$

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\(^3\)Figures 7.6 and 7.7 represent plots of the condensate and thermal density profiles, the LCLS energy versus temperature, and the excitation energy spectrum for the on-axis time-independent solutions in the frame rotating at the extrapolated precessional frequency for the Popov and HFB cases. Comparing these with the corresponding plots in figures 7.1 and 7.2 for the on-axis time-independent solutions in the LAB frame, we note the shift in the quasi-particle excitation energies due to the angular momentum.
Figure 7.5: (a) Precessional frequency $\Omega$ (in units of radial trapping frequency $\omega_r$) versus vortex position $a$ at temperatures $0\text{nK}, 2\text{nK}, 5\text{nK}$ and $7.5\text{nK}$ (triangles, diamonds, circles, squares respectively), (b) Precessional frequency $\Omega$ versus temperature $T$ at vortex positions $0.1, 0.5, 0.8$ and $1.1$ (triangles, diamonds, circles, squares respectively), (c) LCLS energy $\epsilon_{LCLS}$ versus vortex position $a$ at temperatures $0\text{nK}, 2\text{nK}, 5\text{nK}$ and $7.5\text{nK}$ (triangles, diamonds, circles, squares respectively), (d) LCLS energy $\epsilon_{LCLS}$ versus temperature $T$ at vortex positions $0.1, 0.5, 0.8$ and $1.1$ (triangles, diamonds, circles, squares respectively). All distances are in harmonic oscillator units $r_0$, frequencies in units $\omega_r$, and energies in trap units $\hbar \omega_r$. 
calculation using orthogonal HFB corresponding to the energy gap in the HFB energy spectrum and the quantum depletion.

We note from figure 7.5 that there is absolutely no correlation between the precessional frequencies and the LCLS energies, contrary to the claims of [2, 3]. The excitation due to $\epsilon_{LCLS}$ is given by the mode density corresponding to the LCLS mode, and has nothing to do with precession. The precessional frequencies are determined by the conservation of flow (the continuity equation for the condensate density), and hence by equation (7.59). These calculations also predict precession in the same sense as the circulation, as one would expect, contrary to [2, 3].

We note further that $\epsilon_{LCLS}$ varies continuously with $T$, and we see that $\epsilon_{LCLS}|_{T=0}$ is always some small value. Due to quantum depletion $\epsilon_{LCLS} > 0$ always, even at $T = 0$ for HFB and HFB (Popov).

We also find consistency in the condensate fractions between the on-axis and off-axis calculations, and Figure 7.4(c) shows a plot of the condensate fraction $N_c$ versus $T$(nK) for the off-axis case for HFB, and the on-axis case for Popov for a mode cutoff of 100. Additional points are shown for Popov for mode cutoff of 1639. Shown also is $N_c$ versus $T$ for the ideal gas calculations with $T_c \approx 16.7$nK. The predicted transition temperature $T_c$ is calculated according to the calculation [107]

$$k_B T_c^{2D} = \hbar \sqrt{6 \omega_{trap}} N^{1/2}/\pi \quad (7.72)$$

for a radially harmonically trapped 2D Bose gas. The condensate fraction dependence on $T$ is given by

$$F_c = 1 - (T/T_c^{2D})^2. \quad (7.73)$$

The results reveal that the mode cutoff of 100 is sufficient for $T \lesssim 7.5$nK, but the results for $T \gtrsim T_c/2$ become unreliable. At these temperatures, the HFB formalism is unreliable anyway [108], so a cutoff of 100 modes represents an adequate computational investment. At this cutoff, for $T \approx 5$nK, one estimates an error of $\sim 10\%$ in thermal population which does not qualitatively affect our results. We also perform off-axis calculations for triangular and hexagonal vortex arrays. Plots of $\Omega$ versus temperature $T$ at various values

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4The mode cut-off $N_{cut}$ is limited by the number of computational modes as follows: Suppose the quantum numbers $n$ and $l$ are limited to $n = 1, \ldots, N$ and $l = 0, \pm 1, \ldots, \pm M$, then the number of computational modes for the BdGEs is given by $N_{comp} = N(2M + 1) - 1$, and clearly the mode cut-off cannot exceed the number of computational modes, i.e. $N_{cut} \leq N_{comp}$. In most of the computations done here, $N = 10$ and $M = 10$, so $N_{comp} = 209$, and we have chosen $N_{comp} = 100$ to optimise the computational investment. The case of $N_{cut} = 1639$ corresponds to $N = 40$ and $M = 20$. 

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Figure 7.6: On-axis time-independent solutions in the rotating frame for standard HFB in the Popov approximation, (a) condensate density, (b) thermal density at $T = 1\text{nK}$ (solid line) and $T = 5\text{nK}$ (dashed line), (c) LCLS energy versus temperature, and (d) excitation energy spectrum vs angular quantum number $l$ - energies shown increasing with quantum number $n = 0, 1, \ldots$. All distances are in harmonic oscillator units $r_0$, densities in units $N r_0^{-2}$ where $N$ is the number of atoms, and energies in trap units $\hbar \omega_r$.

Figure 7.7: On-axis time-independent solutions in the rotating frame for orthogonal HFB, (a) condensate density, (b) thermal density at $T = 2\text{nK}$ (solid line) and $T = 7.5\text{nK}$ (dashed line), (c) LCLS energy versus temperature, and (d) excitation energy spectrum vs angular quantum number $l$ - energies shown increasing with quantum number $n = 0, 1, \ldots$. All distances are in harmonic oscillator units $r_0$, densities in units $N r_0^{-2}$ where $N$ is the number of atoms, and energies in trap units $\hbar \omega_r$. 

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of lattice parameter $a$ and of $\Omega$ versus lattice parameter $a$ at various values of temperature $T$ are shown in figures 7.9(a),(b) for the triangular vortex array, and in figures 7.10(a),(b) for the hexagonal vortex array. Again from figures 7.9(c),(d) which show plots of $\epsilon_{LCLS}$ versus temperature $T$ at various values of lattice parameter $a$ and of $\epsilon_{LCLS}$ versus lattice parameter $a$ at various values of lattice parameter temperature $T$ for the triangular vortex array, and figures 7.10(c),(d) for the hexagonal vortex array, we see that the precessional frequencies $\Omega$ and the LCLS energies $\epsilon_{LCLS}$ are completely uncorrelated. As in the single vortex case, we note an increase in $\Omega$ with increasing $T$, but only after reaching a minimum at $T \sim 2nK$ in the case of the triangular vortex array, and at $T \sim 5nK$ in the case of the hexagonal vortex array. This increase is also more gradual than in the single vortex case. We note also that $\Omega$ no longer increases with increasing lattice parameter $a$ in contrast with the single off-axis case where $\Omega$ increases with increasing lattice parameter $a$. This may be explained in terms of the areal density law (see discussion on page 167).

Figures 7.11(a)-(c) show, respectively, simulated absorption images for the condensate density, the thermal density, and the condensate phase in the xy-plane for a single off-axis vortex situated at $a = 0.5$. We note the phase singularity in figure 7.11(c) indicating a singly charged vortex. Figures 7.11(d)-(f) show, respectively, simulated absorption images.
Figure 7.9: Triangular vortex array (a) Precessional frequency $\Omega$ (in units of radial trapping frequency $\omega_r$) versus lattice parameter $a$ at temperatures 1nK, 2nK, 5nK and 7.5nK (triangles, diamonds, circles, squares respectively), (b) Precessional frequency $\Omega$ versus temperature $T$ for lattice parameter $1.5\sqrt{3}$, $1.65\sqrt{3}$, $1.8\sqrt{3}$, and $2\sqrt{3}$ (triangles, diamonds, circles, squares respectively), (c) LCLS energy $\epsilon_{LCLS}$ versus lattice parameter $a$ at temperatures 1nK, 2nK, 5nK and 7.5nK (triangles, diamonds, circles, squares respectively), (d) LCLS energy $\epsilon_{LCLS}$ versus temperature $T$ for lattice parameter $1.5\sqrt{3}$, $1.65\sqrt{3}$, $1.8\sqrt{3}$, and $2\sqrt{3}$ (triangles, diamonds, circles, squares respectively). All distances are in harmonic oscillator units $r_0$, frequencies in units $\omega_r$, and energies in trap units $\hbar \omega_r$. 
Figure 7.10: Hexagonal vortex array (a) Precessional frequency $\Omega$ (in units of radial trapping frequency $\omega_r$) versus lattice parameter $a$ at temperatures 1nK, 2nK, 5nK and 7.5nK (triangles, diamonds, circles, squares respectively), (b) Precessional frequency $\Omega$ versus temperature $T$ for lattice parameter 2.75, 2.8, 2.9 and 3 (triangles, diamonds, circles, squares respectively), (c) LCLS energy $\epsilon_{LCLS}$ versus lattice parameter $a$ at temperatures 1nK, 2nK, 5nK and 7.5nK (triangles, diamonds, circles, squares respectively), (d) LCLS energy $\epsilon_{LCLS}$ versus temperature $T$ for lattice parameter 2.75, 2.8, 2.9 and 3 (triangles, diamonds, circles, squares respectively). All distances are in harmonic oscillator units $r_0$, frequencies in units $\omega_r$, and energies in trap units $\hbar\omega_r$. 
for the condensate density, the thermal density, and the condensate phase in the xy-plane for a triangular vortex array having lattice parameter $a = 1.65\sqrt{3}$, and figures 7.11(g)-(i) the respective plots for a hexagonal vortex array having lattice parameter $a = 2.9$. We note the phase singularities in figures 7.10 (f) and (i) indicating respectively, three and seven singly charged vortices. Unfortunately it is not possible to find stationary solutions for the limit of a sufficiently large number of vortices to check out the areal density approximation [109–111]. The areal density approximation is essentially a Thomas-Fermi approximation for the vortex density of a uniform vortex array in a BEC trapped harmonically with a strong uniaxial anisotropy, and is given by

$$\bar{n}_v \approx \frac{\Omega m}{\pi \hbar} - \frac{1}{2\pi} \frac{R_{TF}^2}{(R_{TF}^2 - r^2)^2} \ln \left( \frac{e^{-1}}{\xi^2 \omega_r} \right)$$

(7.74)

for $r \ll R_{TF}$, where $R_{TF}$ is the Thomas-Fermi radius, $\Omega$ is the precessional frequency of the vortex lattice, and $\xi$ is the coherence length [111], and thus we obtain the approximation

$$\Omega \approx \frac{\hbar \pi}{m} \left( \bar{n}_v + \frac{1}{2\pi} \frac{R_{TF}^2}{(R_{TF}^2 - r^2)^2} \ln \left( \frac{e^{-1}}{\xi^2 \omega_r} \right) \right)$$

(7.75)

where the areal density of vortices $\bar{n}_v$ is approximated by $\bar{n}_v \approx N_v / (\pi R_{TF}^2)$, and $N_v$ is the number of vortices in the vortex array.

Figures 7.12 (a) and (b) represent plots of precessional frequency $\Omega$ versus lattice parameter $a$ for vortex arrays composed of two, three and seven vortices at $T = 2nK$ and $T = 5nK$ respectively. We see that $\Omega$ increases with an increasing number of vortices. The inserts of Figures 7.12 (a) and (b) seem to indicate that $\Omega$ tends asymptotically to an upper limit as the number of vortices increases, presumably the limit predicted by the areal density approximation given by (7.75) [111] where $n_v$ is the areal density of vortices approximated by $n_v \approx N_v / (\pi R_{TF}^2)$. Here $N_v$ is the number of vortices in the vortex array, and $R_{TF}$ is the Thomas Fermi radius. In the dimensionless units used here, this may be written

$$\Omega \approx \frac{1}{R_{TF}^2} \left( N_v + \frac{1}{2} \frac{1}{(1 - \frac{r^2}{R_{TF}^2})^2} \ln \left( \frac{e^{-1}}{\Omega} \right) \right)$$

(7.76)

which is, to first approximation, given by $\Omega \approx N_v / (R_{TF}^2)$. Therefore, for the hexagonal array where $N_v = 7$, and taking $R_{TF} \sim 3.5r_0$, we predict to first approximation a precessional frequency of $\Omega \sim 0.57\omega_r$. Taking into account the second term in (7.76) with $r \sim 0.5R_{TF}$, we predict $\Omega \sim 0.55\omega_r$ (so the second term is unimportant in the regime considered here).

This is of the order of 20% lower than the value predicted using the continuity equation for the condensate density calculation. We note that the areal density approximation is
Figure 7.11: Simulated absorption images [116] for off-axis vortex, triangular vortex array and hexagonal vortex array showing (a) condensate density, (b) thermal density, (c) condensate phase for a single vortex at \( a = 0.5 \) and (d) condensate density, (e) thermal density, (f) condensate phase for a triangular vortex array with lattice parameter \( a = 1.65\sqrt{3} \), and (g) condensate density, (h) thermal density, (i) condensate phase for a hexagonal vortex array with lattice parameter \( a = 2.9 \). All positions are in units of the oscillator length \( r_0 \).
Figure 7.12: Precessional frequency $\Omega$ versus lattice parameter $a$ for vortex arrays composed of two (circles), three (triangles) and seven vortices (squares) with cubic spline interpolation (dashed line) (a) at $T = 2nK$, and (b) at $T = 5nK$. The insert in each respective figure shows the precessional frequency $\Omega$ versus number of vortices for vortex arrays composed of two, three and seven vortices having lattice parameter $a = 3.0$ with cubic spline interpolation (dashed line). All frequencies are in units of the radial trapping frequency $\omega_r$. All positions are in units of the oscillator length $\rho_0$.

only valid for a large number of vortices. Furthermore the inserts of figures 7.12 (a) and (b) reveal that the precessional frequency approaches an asymptotic value of $\sim .72$. We conclude, however, that these results are consistent in the asymptotic limit.

The areal density law (7.75) may also be used to explain the fact that $\Omega$ increases with increasing lattice parameter $a$ for the cases of the triangular and hexagonal vortex arrays over the range shown (within the Thomas-Fermi radius), and may be understood by considering that the vortex precessional velocity is determined by the background velocity field around the vortex core, and the core shape [112, 113]. The effect of their image charge in the condensate boundary is less important, in contrast with the single vortex case [114, 115]. In the single off-axis vortex case, $\Omega$ increases with increasing $a$. This is in agreement with GPE results [114, 115], and may be explained in terms of the effect of the vortex’s image charge in the boundary of the condensate [114, 115].

### 7.4.4 Equivalence of Single Vortex Case with Multistate Model

Since the multi-state model and the continuity equation for the condensate density predictions for the precessional frequency of a single off-axis vortex both imply particle number
conservation, and the construction of the vortex state in the multi-state is from a complete basis set, and is therefore completely general for the vortex state, one would expect the two methodologies to yield the same result in the limit of no energy cut-off. Here we shall demonstrate that this is indeed the case, and that the two representations are exactly equivalent. From (7.49), we see that the time independent solution for the multistate model in the rotating frame is given by

\[ \Phi_{MS}(r, \theta) = a_g \sum_{l \neq 1} \phi_g^{(l)}(r) \frac{e^{i l \theta}}{\sqrt{2\pi}} + a_v \phi_v(r) \frac{e^{i \theta}}{\sqrt{2\pi}} \]  

(7.77)

and for the vortex calculation above by (7.66)

\[ \Phi_{VC}(r, \theta) = \sum_{l, n \in S^{(1)}} a_{ln} \chi_{ln}^{(1)}(r, \theta) \]  

(7.78)

where \( \chi_{ln}^{(1)}(r, \theta) \) is given by (7.64). The expression for \( \Phi_{VC}(r, \theta) \) given by (7.78) can be rewritten as

\[ \Phi_{VC}(r, \theta) = \sum_{l \neq 1} \left( \sum_n a_{ln} \xi_{ln}(r, \theta) \right) \frac{e^{i l \theta}}{\sqrt{2\pi}} + \left( \sum_n a_{ln} \xi_0(n, r, \theta) - \sum_{l \neq 1} \sum_n a_{ln} \Lambda_{ln}^{(1)} \xi_{10}(r, \theta) \right) \frac{e^{i \theta}}{\sqrt{2\pi}} \]  

(7.79)

where \( \Lambda_{ln}^{(1)} \equiv \xi_{ln}(r_1, \theta_1)/\xi_{10}(r_1, \theta_1) \) for a single off-axis vortex situated at position \( (r_1, \theta_1) \). Comparing expression (7.77) with (7.79), we can identify

\[ a_g \phi_g^{(l)}(r) \equiv \sum_n a_{ln} \xi_{ln}(r, \theta) \]  

(7.80)

and

\[ a_v \phi_v(r) \equiv \sum_n a_{ln} \xi_0(n, r, \theta) - \sum_{l \neq 1} \sum_n a_{ln} \Lambda_{ln}^{(1)} \xi_{10}(r, \theta) \]  

(7.81)

showing that the two representations are equivalent for a single vortex. We use equation (7.58) to calculate the precessional frequency \( \Omega_{MS} \) as predicted by the multi-state model with the corresponding precessional frequency calculated using the continuity equation for the condensate density, equation (7.59) for mode cut-off of 100, and of 209. These are plotted in figure 7.13, and we see that for a sufficient mode cut-off, the agreement is excellent.

### 7.5 Two-dimensional Time-dependent Simulations

All time-dependent solutions are done in the interaction picture. We write (ignoring \( \Delta \mu \), i.e the shift in the chemical potential due to the fugacity for a finite number of atoms - see
Figure 7.13: Comparison of precessional frequencies $\Omega$ as predicted by orthogonal HFB (circles) with precessional frequencies $\Omega_{MS}$ as predicted by the multi-state model (squares), (a) for a mode cut-off of 100, and (b) for a mode cut-off of 209. (All frequencies in units of radial trapping frequency $\omega_r$).

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\begin{align*}
\Phi(r, t) &= \Phi'(r, t) \exp(-i\mu t/\hbar) \quad (7.82) \\
u_q(r, t) &= u'_q(r, t) \exp(-i\epsilon_q t/\hbar) \\
v_q(r, t) &= v'_q(r, t) \exp(-i\epsilon_q t/\hbar) \quad (7.83)
\end{align*}

Then

\[ i\hbar \frac{\partial}{\partial t} \Phi(r, t) = \left( i\hbar \frac{\partial}{\partial t} \Phi'(r, t) + \mu \Phi'(r, t) \right) \exp(-i\mu t/\hbar) \]

and writing the anomalous density $\tilde{m}(r, t)$ as

\[ \tilde{m}(r, t) = \tilde{m}'(r, t) \exp(-2i\mu t/\hbar) \]

we find, dropping the primes for notational convenience, that the orthogonal time-dependent GGPE in the interaction picture is given by

\[ i\hbar \frac{\partial \Phi(r, t)}{\partial t} = \left( \hat{h} - \mu + g (|\Phi|^2 + 2\tilde{m}) \right) \Phi(r, t) + g\tilde{m}\Phi^*(r, t) - \int dr' \hat{P}(r', r') \phi(r') \quad (7.84) \]

From (7.83)

\[ i\hbar \frac{\partial u_q(r, t)}{\partial t} = \left( i\hbar \frac{\partial u'_q(r, t)}{\partial t} + \epsilon_q u'_q(r, t) \right) \exp(-i\epsilon_q t/\hbar) \]

and

\[ i\hbar \frac{\partial v_q(r, t)}{\partial t} = \left( i\hbar \frac{\partial v'_q(r, t)}{\partial t} + \epsilon_q v'_q(r, t) \right) \exp(-i\epsilon_q t/\hbar) \]

so the BdGEs in the interaction picture are (dropping the primes for notational convenience)

\[ i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r, r', t, -\epsilon_q) & \hat{M}(r, r', t) \\ -\hat{M}^*(r, r', t) & -\hat{L}^*(r, r', t, \epsilon_q) \end{bmatrix} \begin{bmatrix} u_q(r', t) \\ v_q(r', t) \end{bmatrix}. \quad (7.85) \]
where

\[ \hat{L}(r, r', t, \epsilon_q) \equiv \hat{L}(r, r', t) + \epsilon_q \delta(r - r') \]  

(7.86)

As pointed out in chapter 4, \( \Delta \mu \) is negligible in the temperature regime of interest, and can be ignored. Initially all standard HFB time-dependent simulations were done using the RK4IP algorithm [90, 105] (see chapter 5, sections 5.4.1, 5.4.2 for a summary), but with the need to implement the orthogonal formalism\(^5\) (7.84) and (7.85), a new fourth order Runge-Kutta algorithm based on the evolution of the coefficients of the condensate wave function, and of the quasiparticle amplitudes expanded in the Laguerre basis was implemented (see chapter 5, section 5.4.3 for a description of the algorithm). This algorithm has the advantage that it permits a much larger energy cut-off, and also runs quicker, in view of the Gaussian grid which is much smaller than the Fourier grid required for the RK4IP algorithm - see chapter 5, section 5.4.3 for a comparison. The results obtained with each method are comparable - see chapter 5, section 5.4.3 on numerical methods.

### 7.5.1 Evolution of Time-independent Solutions

Time-dependent simulations were done for the standard HFB for \( T = 5\)nK for a vortex at \( a = 0.5 \) radial harmonic oscillator units from the axis, with a mode cutoff of 100, using the time-independent data initial state. In all the simulations, the vortex precession describes a circle. The precessional frequency was estimated using a least squares fit of a sinusoid to the vortex x-displacement versus time, and was found to be \( \Omega_{\text{LS}} = 0.3794\omega_r \), in good agreement with the value of \( \Omega = 0.3727\omega_r \), as predicted in the time-independent calculations. The error in the prediction scales as the number of computational basis functions\(^6\) which, for practical reasons, is only 209 in these calculations. Calculations for the single off-axis vortex taking the projector \( \hat{P} \) into account, presented in appendix F.3 predict a value of \( \Omega = 0.3756\omega_r \). For 839 computational basis functions, the time-independent calculations predict a value of \( \Omega = 0.3761\omega_r \). We see no evidence of dissipation during the time of the simulation of ten trap cycles. Examination of the plot of the x-displacement versus time (in trap cycles) in figure 7.14(a) reveals that this is indeed the case. Figure 7.14(b) shows that the trajectory of the vortex constitutes a circle.

\(^5\)See comments on use of standard time-dependent HFB versus orthogonal time-dependent HFB at end of section 5.4.

\(^6\)Clearly it would be desirable to increase the mode cut-off. However, for practical reasons, these are limited to 100, since these results are still reasonably accurate (\( \sim 2\% \)) and to increase this number would significantly increase the computational effort, rendering these calculations impractical. These results can be refined, but the computation required is formidable.
Time-dependent simulations were also done for the standard HFB for $T = 5\mu K$ for a symmetrical triangular vortex array with lattice parameter $\alpha = 1.65\sqrt{3}$ (i.e. three vortices symmetrically positioned at 1.65 radial harmonic oscillator units from the axis), and for a symmetrical hexagonal triangular vortex centred on the axis having lattice parameter $\alpha = 2.85$ (i.e. seven vortices), again using time-independent calculations for the initial state. For this symmetric case, all vortices precess in the same way with phase differences of $2\pi/3$ and $\pi/3$ for the triangular and hexagonal vortex arrays respectively, with the exception of the central vortex in the hexagonal array, which remains fixed. In both simulations, the vortex precession describes a circle. Again we see no evidence of dissipation during the time of the simulation of five trap cycles. Examination of the plots of the $x$-displacement versus time (in trap cycles) in figures 7.14(c) and 7.14(e), where we have selected a representative vortex for display purposes, reveals that this is indeed the case. The precessional frequency for the triangular vortex array was estimated using a least squares fit of a sinusoid to the vortex $x$-displacement versus time of a representative vortex, and was found to be $\Omega_{LS} = 0.5856\omega_r$, in good agreement with the value of $\Omega = 0.5938\omega_r$, as predicted in the time-independent calculations for 209 computational basis functions. Figures 7.14(d) and 7.14(f) show, respectively the trajectories of the representative vortices, which both constitute a circle.

### 7.5.2 Stirring of the Condensate

In these simulations we use one or more Gaussian stirrers in order to stir the condensate. The stirring imparts angular momentum to the condensate, and therefore one would expect the production of vortices in cases where the angular frequency of the stirrer(s) exceeds a certain critical value. This should correspond (at least approximately) to the velocity of the stirrer with respect to the stirrer exceeding the local Landau critical velocity (i.e. the local speed of sound). In what follows we shall establish a critical stirring frequency, below which no vortices are produced in regions of appreciable density (i.e. within the Thomas-Fermi radius). In these simulations we find that this critical frequency corresponds to a velocity of the stirrer through the BEC that is slightly in excess of the local Landau critical velocity\(^7\) (see table 7.1).

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\(^7\)This may be explained by noting the following: The expression $s = \sqrt{ng/m}$ for the “speed of sound” is that appropriate to the Bogoliubov approximation (and the HFB-Popov approximation). In the HFB case, however, the spectrum is steepened by the presence of the anomalous density (see equation (44) of Griffin [11]), and is not linear in $k$ as $k \to 0$ anyway, due to the presence of the gap. Thus the critical velocity obtained from the fundamental Landau definition $V_c = \min (E(k)/k)$ will be raised above the
Figure 7.14: Vortex precessional motion for single off-axis vortex with lattice parameter $a = 0.5$ showing (a) $x$-displacement of vortex versus time, (b) vortex trajectory, for triangular vortex array with lattice parameter $a = 1.65\sqrt{3}$ showing (c) $x$-displacement of representative vortex versus time, (d) trajectory for representative vortex, and for hexagonal vortex array with lattice parameter $a = 2.85$ showing (e) $x$-displacement of representative vortex versus time, and (f) trajectory for representative vortex.
In the simulations where the critical stirring frequency is exceeded, we are able to determine by the method of least squares, the precessional frequencies and compare these with the values predicted in the time-independent calculations using the continuity equation for the condensate density. We shall see presently that the agreement between the time-dependent values and the predicted values using the time-independent calculations is good, as one would expect in the quasi-static case since then the term \( i\hbar \frac{\partial}{\partial t} |\Phi|^2 \) in the time-dependent continuity equation for the condensate density (4.110) is small. In the first three simulations a single Gaussian stirrer was used to stir the BEC. In the fourth simulation, three symmetrically placed Gaussian stirrers were used.\(^8\) The Gaussian potential corresponding to a stirrer of amplitude \( A_0 \) and FWHM \( 2\sqrt{\ln 2}s_s \), rotating at angular stirring frequency \( \Omega_s \), initially at position \((r_s, \theta_s)\) is given by

\[
V_s(r, \theta, t) = A_0 \exp \left[ - \left( \frac{(r \cos \theta - r_s \cos (\theta_s + 2\pi \Omega_s t))^2 + (r \sin \theta - r_s \sin (\theta_s + 2\pi \Omega_s t))^2}{s_s^2} \right) \right].
\]

Where multiple stirrers are employed, the stirring potential is merely the sum of each Gaussian stirrer. In each simulation, the initial ground state solution was found using the time-independent HFB equations with the Gaussian stirrer(s) already in place. In all cases, no vortices were present in the initial state, and the Gaussian stirrers were all situated at \( a=1.5r_0 \) off axis, of amplitude \( 10\hbar \omega_r/2 \) (i.e. of the same order as the chemical potential \( \mu \sim 10\hbar \omega_r/2 \)), full width half maximum (FWHM) \( 0.82r_0 \), and were initially at rest, and the stirring frequency ramped up from zero to the required angular frequency \( \Omega_s \) over a period of 0.2 trap cycles. The four sets of simulations were as follows:

1. A single Gaussian stirrer on for 10 trap cycles, \( \Omega_s = 0.38\omega_r \).
2. A single Gaussian stirrer on for 2.5 trap cycles, \( \Omega_s = 0.5\omega_r \).
3. A single Gaussian stirrer on for 4.5 trap cycles, \( \Omega_s = 0.5\omega_r \).
4. Three equi-spaced Gaussian stirrers on for 2.5 trap cycles, \( \Omega_s = 0.5\omega_r \).

In the case of the first simulation, the rotational frequency \( \Omega_s \) is sub-critical, so no vortices are produced within the Thomas Fermi radius, therefore negligible angular momentum is Bogoliubov speed of sound \( s \), due to both the steepening of the spectrum and the finite gap.

\(^8\)The reason for using three Gaussian stirrers, as opposed to just one, is not that we need three stirrers to create three vortices (one stirrer is sufficient for this purpose provided the BEC is stirred long enough at a sufficiently high frequency), but rather in order to create a symmetrical triangular vortex array so that the time-independent predictions can be tested.
Figure 7.15: (Colour on-line) Stirring of condensate showing (a) z-component of total angular momentum (solid black line), condensate angular momentum (dashed blue line), and thermal population angular momentum (dash-dotted red line) versus time, (b) change in thermal population $\Delta N_t(t) - \Delta N_t(0)$ versus time, and (c) change in condensate population $\Delta N_c(t) - \Delta N_c(0)$ versus time. In cases I-III the condensate is stirred at frequencies $0.38 \omega_r$, $0.5 \omega_r$, and $0.5 \omega_r$ for 10, 2.5 and 4.5 trap cycles respectively using a single Gaussian stirrer. In case IV the condensate is stirred at $0.5 \omega_r$ for 4.5 trap cycles using three equi-spaced Gaussian stirrers. All Gaussian stirrers are situated at $a = 1.5 r_0$ off axis, are of amplitude $10 \hbar \omega_r / 2$, FWHM $0.82 r_0$, and are switched on adiabatically over 0.2 trap cycles. The change in the populations $\Delta N_t$ and $\Delta N_c$ are given in units of $N$. All angular momenta are in units of $N \hbar$. 


Figure 7.16: Simulated absorption images [116] - stirring of condensate in an anti-clockwise direction using one Gaussian stirrer at \( a = 1.5r_0 \) off axis, of amplitude \( 10\hbar \omega_r/2 \), FWHM \( 0.82r_0 \), switched on adiabatically over 0.2 trap cycles, stirring frequency \( 0.5\omega_r \), stirrer on for 2.5 trap cycles after (a) 0.5, (b) 1, (c) 1.5, (d) 2, (e) 2.5, (f) 3, (g) 3.5, (h) 4, (i) 4.5, (j) 5, (k) 5.5, (l) 6, (m) 6.5, (n) 7, (o) 7.5, (p) 8, (q) 8.5, (r) 9, (s) 9.5, and (t) 10 trap cycles. All positions are in units of the harmonic oscillator length \( r_0 \).
Figure 7.17: Simulated absorption images [116] - stirring of condensate in an anti-clockwise direction using one Gaussian stirrer at $a = 1.5r_0$ off axis, of amplitude $10\hbar\omega_r/2$, FWHM $0.82r_0$, switched on adiabatically over 0.2 trap cycles, stirring frequency $0.5\omega_r$, stirrer on for 4.5 trap cycles after (a) 0.5, (b) 1, (c) 1.5, (d) 2, (e) 2.5, (f) 3, (g) 3.5, (h) 4, (i) 4.5, (j) 5, (k) 5.5, (l) 6, (m) 6.5, (n) 7, (o) 7.5, (p) 8, (q) 8.5, (r) 9, (s) 9.5, and (t) 10 trap cycles. All positions are in units of the harmonic oscillator length $r_0$. 
Figure 7.18: Simulated absorption images [116] - stirring of condensate in an anti-clockwise direction using three equi-spaced Gaussian stirrers at $a = 1.5r_0$ off axis, of amplitude $10\hbar \omega r/2$, FWHM $0.82r_0$, switched on adiabatically over 0.2 trap cycles, stirring frequency $0.5\omega_r$, stirrer on for 2.5 trap cycles after (a) 0.5, (b) 1, (c) 1.5, (d) 2, (e) 2.5, (f) 3, (g) 3.5, (h) 4, (i) 4.5, (j) 5, (k) 5.5, (l) 6, (m) 6.5, (n) 7, (o) 7.5, (p) 8, (q) 8.5, (r) 9, (s) 9.5, and (t) 10 trap cycles. All positions are in units of the harmonic oscillator length $r_0$. 

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Figure 7.19: Stirring of condensate - (I) using one Gaussian stirrer at stirring frequency $0.5\omega_r$ for 2.5 trap cycles (a) x-displacement of vortex, (b) y-displacement of vortex, and (c) trajectory of vortex over a period of ten trap cycles, (II) using one Gaussian stirrer at stirring frequency $0.5\omega_r$ for 4.5 trap cycles (a) x-displacement of vortex 1, (b) y-displacement of vortex 1, and (c) trajectory of vortex 1 over a period of ten trap cycles (d) x-displacement of vortex 2, (e) y-displacement of vortex 2, and (f) trajectory of vortex 2 over a period of ten trap cycles, (III) using three equi-spaced Gaussian stirrers at stirring frequency $0.5\omega_r$ for 2.5 trap cycles (a) x-displacement of vortex 1, (b) y-displacement of vortex 1, and (c) trajectory of vortex 1 over a period of ten trap cycles (d) x-displacement of vortex 2, (e) y-displacement of vortex 2, and (f) trajectory of vortex 2, and (g) x-displacement of vortex 3, (h) y-displacement of vortex 3, and (i) trajectory of vortex 3 over a period of ten trap cycles. All Gaussian stirrers are situated at $a = 1.5r_0$ off axis, are of coupling strength $10\hbar\omega_r/2$, FWHM $0.82r_0$, and are switched on adiabatically over 0.2 trap cycles. All positions are in units of the harmonic oscillator length $r_0$. 
transferred to the condensate. This angular momentum is due to circulation corresponding to vortices in regions of negligible density. A small amount of angular momentum is also transferred to the thermal cloud. This accounts for the small amount of angular momentum in the condensate and in the thermal population as shown in figure 7.15 I(a) which is a plot of the z-component of the angular momentum versus time. We note that $L_z$ remains fixed once the stirring ceases after 10.2 trap cycles in accordance with the conservation of angular momentum. We note that the angular momentum for the thermal population increases for the first few trap cycles, reaching a saturation value after $\sim 4 \rightarrow 5$ trap cycles. Simulations over a much longer time scale (not presented here) reveal a slow cyclical change in the thermal population angular momentum of a few percent. Once the stirrer is switched off, we see a steady increase in the thermal population angular momentum with a resultant loss in the angular momentum of the condensate (since the overall angular momentum is conserved). During the time of stirring, the condensate angular momentum varies cyclically corresponding to the variation of vortices from the axis (see also [90, 105]). In the case where the stirring frequency is sub-critical, these vortices would lie outside the Thomas Fermi radius and would therefore be sub-threshold. Figures 7.15 I(b),(c) show respectively the changes in condensate and thermal density, where we see rigorous observance of particle number conservation. In simulations two and three, the stirring frequency $\Omega_s$ is sufficient for the production of vortices, and figures 7.16 (a)-(t) and figures 7.17 (a)-(t) show the respective simulated absorption images. Figures 7.18 (a)-(t) represent simulated absorption images for the fourth simulation using three Gaussian stirrers. In the second sequence, only one vortex is created, and its x-displacement $x_{\text{pos}}$ and y-displacement $y_{\text{pos}}$ versus time in trap cycles shown in figures 7.19 I(a),(b), and its trajectory in figure 7.19 I(c) [117]. In all four cases we see evidence of heating as the condensate is stirred in figure 7.15 in panels I(b), II(b), III(b), and IV(b), which each indicate an increase in the thermal population. In order to understand why there exists a critical frequency for the production of vortices within the Thomas Fermi radius, we calculate the Landau critical velocity $v_{\text{LC}}$ given by the speed of sound at the point of the stirrer $s = \sqrt{ng/m}$ where $n$ is the density of the superfluid, and $m$ is the mass of a particle. We use the local density approximation, and calculate the speed of sound $s$ at the stirrer using the local density $n$ of the superfluid at the point of the stirrer.

In these simulations, we measure the two-dimensional density $n^{(2D)}$ where we have inte-
Table 7.1: Relationship of the local stirrer velocity with the average z-component of the angular momentum $\bar{L}_z$ for time-dependent HFB simulations.

<table>
<thead>
<tr>
<th>$\Omega(\omega_r)$</th>
<th>$n^{(2D)}(r_0^{-2})$</th>
<th>$v_{\text{stir}}/v_{LC}$</th>
<th>$\bar{L}_z(N\hbar)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.38</td>
<td>0.02</td>
<td>1.12</td>
<td>0.035</td>
</tr>
<tr>
<td>0.39</td>
<td>0.02</td>
<td>1.15</td>
<td>0.045</td>
</tr>
<tr>
<td>0.4</td>
<td>0.02</td>
<td>1.18</td>
<td>0.5 (varies between $\sim 0.25$ and $\sim 0.7$)</td>
</tr>
<tr>
<td>0.45</td>
<td>0.02</td>
<td>1.33</td>
<td>0.55 (varies between $\sim 0.3$ and $\sim 0.8$)</td>
</tr>
<tr>
<td>0.5</td>
<td>0.02</td>
<td>1.48</td>
<td>0.6 for one vortex, $\sim 0.8$ for two vortices and $\sim 2.2$ for three vortices</td>
</tr>
</tbody>
</table>

Table 7.1: Relationship of the local stirrer velocity with the average z-component of the angular momentum $\bar{L}_z$ for time-dependent HFB simulations.
II(a), (b), and 7.19 II(d), (e), and the trajectories in figure 7.19 II(c) and 7.19 II(f). Figures 7.15 II(a) and 7.15 III(a) show the z-component of the angular momentum as the stirring process ensues, showing that the z-component of the angular momentum is conserved once the stirring is stopped.

No experiments have been performed on stirring a BEC using a narrow rotating probe as considered here but experiments [42] have been performed which show evidence of a critical stirring angular velocity using elliptical deformation of the trap. These experiments also show jumps in the z-component of the angular momentum due to additional vortices, consistent with the results here, even when one takes into consideration the fact that the angular momentum also depends on the distance of the vortex from the axis, and therefore may vary appreciably depending on the configuration of the vortices. Experiments to test the superfluid critical velocity using the linear motion of a narrow probe laser beam have also been performed [118–120], finding critical velocities for the onset of dissipation $\sim 5-10$ times smaller than the critical velocity inferred from the bulk Bogoliubov speed of sound.

Time-dependent GPE simulations [121] also indicate that dissipation first occurs at speeds significantly less than the speed of sound. However, the linear motion of the probe in these works excite vortex dipole or solitons, and are not therefore directly applicable to the present work.

In a previous study [90, 105], similar stirring simulations were carried out using time-dependent GPE simulations. However, the critical stirring frequency referred to in these results are the thermodynamic critical frequency (at which the vortex-free and central vortex states have equal energies), whereas the results presented here refer to the critical frequency at which vortices are created within the Thomas Fermi radius. Nevertheless, the results of [90, 105] are consistent with the simulations performed in this work.

One can also explain the existence of a critical stirring angular frequency in terms of the GPE ground state solution [98]. In the LAB frame the ground state is always of lower energy than the vortex state, therefore we find no vortices in an unstirred condensate. In the absence of interactions, the energies of the ground state ($l = 0$) and the vortex state ($l = 1$) are given by the single-particle solutions $\hbar \omega_r$ and $2\hbar \omega_r$ respectively. For a condensate stirred at angular frequency $\Omega$ the $l = 1$ single particle energy is given by $\hbar \omega_r (1 - \Omega/\omega_r)$, and therefore these energies are the same at $\Omega = \omega_r$. In the interacting gas with (weak) repulsive interactions, however, there exists a critical frequency $\Omega_c < \omega_r$ above which the vortex ($l = 1$) state has a lower energy than the $l = 0$ state, and is therefore the ground state.
Figures 7.18 (a)-(t) show the creation of three vortices in the fourth simulation, and the x-displacement and y-displacement versus time in trap periods for representative vortices are shown in figures 7.19 III(a),(b), 7.19 III(d),(e), and 7.19 III(g),(h) respectively, and the trajectories in figures 7.19 III(c), 7.19 III(f), and 7.19 III(i). The least squares estimates of the precessional frequency of $\Omega_{LS} = 0.68\omega_r$, are in good agreement with the interpolated values from figures 7.9 (a) and (b) of $\Omega \sim 0.65\omega_r$.

The above results for the stirring simulations indicate good agreement with the values predicted using the continuity equation for the condensate density in the time-independent calculations. These results were attained in the case where the stirrers were introduced adiabatically. One would expect differences in the precessional frequencies in the case where the introduction of the stirrers is non-adiabatic, and that the time-independent predictions would be approximate since the term $i\hbar \frac{\partial}{\partial t} |\Phi|^2$ in the continuity equation for the condensate density (4.110) is then important.

### 7.5.3 Breaking of the Axial Symmetry of the Trapping Potential

Noether’s theorem [122] states that in a conservative physical system, a differentiable symmetry of the Lagrangian (and it can be shown, of the Hamiltonian) has a conserved quantity associated with the system (i.e a corresponding conservation law). In this case the axial symmetry of the trapping potential implies the conservation of the axial component (i.e the z-component) of the angular momentum, as is indicated by (4.122)

$$\frac{d \langle L \rangle}{dt} = \int d\mathbf{r} \left(|\Phi|^2 + \bar{n}\right) \mathbf{L} V_T$$

(7.90)

which determines the rate of change in angular momentum in the BEC system, where we see that $d \langle L_z \rangle / dt = 0$ for an axially symmetric trapping potential. The implication of this is that when this symmetry is broken, $\langle L_z \rangle$ is no longer conserved, and since there is no external source of angular momentum here, we conclude that angular momentum will be lost since $d \langle L_z \rangle / dt$ will now be non-zero by equation (7.90). This leads to vortex decay, and the vortex spirals outwards as angular momentum is lost. This is in accordance with work done by Zhuravlev et. al. [123] on the arrest of vortex arrays by a trap anisotropy, although this work deals with large vortex arrays, whereas the calculations performed here concern single off-axis vortices and small vortex arrays. In order to test this prediction, we introduce adiabatically an eccentricity into the trapping potential, thereby breaking the axial symmetry. The eccentricity was introduced by means of the perturbation potential

$$V_{\text{pert}}(r, \theta) = \epsilon r^2 \left(\sin^2 \theta - \cos^2 \theta\right)$$

(7.91)
which is introduced adiabatically after two trap cycles over either five or twenty trap cycles, depending on the simulation run. The angular momentum is calculated using equation (4.58), viz.

\[
\langle \hat{L} \rangle = i\hbar \int dr \left[ \Phi^* (r \times \nabla) \Phi + \sum_q \left( n_q u_q^* (r \times \nabla) u_q + (n_q + 1) v_q (r \times \nabla) v_q^* \right) \right].
\] (7.92)

Four simulations are performed for symmetry-breaking of the trapping potential. Initially the trapping potential is axially symmetric, and the eccentricity ramped on after two trap cycles over a specified number of trap cycles. The simulations are as follows:

1. The eccentricity is ramped up to \( \epsilon = 0.25 \) over a period of five trap cycles.
2. The eccentricity is ramped up to \( \epsilon = 0.25 \) over a period of twenty trap cycles.
3. The eccentricity is ramped up to \( \epsilon = 0.1 \) over a period of five trap cycles.
4. The eccentricity is ramped up to \( \epsilon = 0.1 \) over a period of twenty trap cycles.

In all cases the BEC initially has a vortex situated at position \( a = 1.1 \) trap units from the axis. The \( z \)-component of the angular momentum \( L_z \) is plotted for all four simulations in figures 7.20 I(a), 7.20 II(a), 7.20 III(a), and 7.20 IV(a) respectively. Figures 7.20 I(b),(c), 7.20 II(b),(c), 7.20 III(b),(c), and 7.20 IV(b),(c) show the respective changes in the thermal and condensate densities, and reveal an increase in the thermal density as the vortex spirals outwards and finally decays. This is consistent with the notion that the vortex decays into excitations when it reaches the condensate boundary [124]. Simulated absorption images for \( \epsilon = 0.25 \) with turn-on time of twenty trap cycles are shown in figures 7.21(a)-(t). The vortex trajectories for the respective simulations are shown in figures 7.22 I(a)-(f), 7.22 II(a)-(f), 7.22 III(a)-(f), and 7.22 IV(a)-(f). In the simulations with \( \epsilon = 0.25 \) the lifetime of the vortex is approximately 145 to 150 trap cycles, and for \( \epsilon = 0.1 \) substantially larger, with an extrapolated value of the order of 700 trap cycles. The vortex precessional frequencies are in good agreement with the time-independent calculations, and we note that in all cases from the vortex trajectories that the vortices precess faster as they move outwards\(^{10}\) which, again, is in agreement with the time-independent results (see figure 7.5(a)), before finally decaying. At this stage, most of the angular momentum associated with the vortex has

\(^{10}\)This is a well-known property of the solution of the GPE [114,115], provided one is away from the Lowest-Landau-Level limit. It is interesting to note that this behaviour persists at finite temperature in the HFB solutions.
been lost, and disappears altogether once the vortex leaves the condensate. As discussed above, this loss of angular momentum is due to the symmetry-breaking of the trap, and the loss of the angular momentum is as given by (7.90). We see from figures 7.21 and 7.22 II in the case where the eccentricity $\epsilon = 0.25$ is introduced over twenty trap cycles, that the vortex is lost after $\sim 145 \rightarrow 150$ trap cycles (loss of tracking after $\sim 146$ trap cycles) which is consistent with the decline in $L_z$ seen in figure 7.20 II(a) and the sudden increase in thermal density in figure 7.20 II(b) at $\sim 145$ trap cycles. These results are also in qualitative agreement with recent simulations using a classical field treatment comprising the projected Gross-Pitaevskii equation [125].

Similar simulations were performed for the triangular vortex array with lattice parameter $a = 1.65\sqrt{3}$, the simulations being as follows:

1. The eccentricity is ramped up to $\epsilon = 0.25$ over a period of five trap cycles.
2. The eccentricity is ramped up to $\epsilon = 0.25$ over a period of twenty trap cycles.
3. The eccentricity is ramped up to $\epsilon = 0.1$ over a period of five trap cycles.
4. The eccentricity is ramped up to $\epsilon = 0.1$ over a period of twenty trap cycles.

The angular momentum calculated using equation (7.92) is plotted in figures 7.23 I(a), II(a), III(a), and IV(a) for simulations 1, 2, 3, and 4 respectively, and indicate a loss of angular momentum as predicted. Figures 7.23 I(b),(c) , 7.23 II(b),(c), 7.23 III(b),(c), and 7.23 IV(b),(c) show the respective changes in the thermal and condensate densities, and reveal increases in thermal density as each successive vortex spirals outwards and finally decays. This corresponds to the slight drop in the angular momentum at these times as indicated in figures 7.23 I(a) , 7.23 II(a), 7.23 III(a), and 7.23 IV(a). The simulated absorption images for $\epsilon = 0.25$ with turn-on time of twenty trap cycles shown in figures 7.24(a)-(t). The vortex trajectories for the respective simulations shown in figures 7.25 I(a)-(i), 7.25 II(a)-(i), 7.25 III(a)-(i), and 7.25 IV(a)-(i) confirm the decay of these vortices. We note the decrease in the precessional frequencies of the remaining vortices following the departure of a vortex in agreement with the time-independent predictions for vortex arrays shown in figure 7.12, which shows the dependence of the precessional frequencies of the vortex array on the lattice parameter for the cases of three vortices (our initial configuration), and of two vortices, and also with figure 7.9(a) which gives the time-independent prediction for the triangular vortex array at various temperatures and values of lattice parameter. The prediction here is $\Omega \sim 0.6\omega_r$ for lattice parameter $a \sim 1.65\sqrt{3} = 2.85$, and is
Figure 7.20: (Colour on-line) Breaking of axial symmetry for single off-axis vortex showing (a) $z$-component of total angular momentum (upper black line) and condensate angular momentum (lower blue line) versus time, (b) change in thermal population $N_t(t) - N_t(0)$ versus time, and (c) change in condensate population $N_c(t) - N_c(0)$ versus time for (I) eccentricity parameter $\epsilon=0.25$ and turn-on time of five trap cycles, (II) eccentricity parameter $\epsilon=0.25$ and turn-on time of twenty trap cycles (see simulated absorption image in figure 7.21), (III) eccentricity parameter $\epsilon=0.1$ and turn-on time of five trap cycles, and (IV) eccentricity parameter $\epsilon=0.1$ and turn-on time of twenty trap cycles. The change in the populations $\Delta N_t$ and $\Delta N_c$ are given in units of the number of atoms $N$. All angular momenta are in units of $Nh$. 
Figure 7.21: Simulated absorption images [116] for breaking of axial symmetry with turn-on time of twenty cycles for single off-axis vortex for eccentricity parameter $\epsilon=0.25$ after (a) 8, (b) 16, (c) 24, (d) 32, (e) 40, (f) 48, (g) 56, (h) 64, (i) 72, (j) 80, (k) 88, (l) 96, (m) 104, (n) 112, (o) 120, (p) 128, (q) 136, (r) 144, (s) 152, and (t) 160 trap cycles. All positions are in units of the harmonic oscillator length $r_0$. 
Figure 7.22: Breaking of axial symmetry for single off-axis vortex for (I) turn-on time of five trap cycles for eccentricity parameter $\epsilon=0.25$, (II) for turn-on time of twenty trap cycles for eccentricity parameter $\epsilon=0.25$ (see simulated absorption image in figure 7.21), (III) for turn-on time of five trap cycles for eccentricity parameter $\epsilon=0.1$, and (IV) for turn-on time of twenty trap cycles for eccentricity parameter $\epsilon=0.1$ showing (a) $x$-displacement of vortex between 0 and 25 trap cycles, (b) $y$-displacement of vortex between 0 and 25 trap cycles, (c) vortex trajectory of vortex between 0 and 25 trap cycles, and (d) $x$-displacement of vortex between 125 and 150 trap cycles, (e) $y$-displacement of vortex between 125 and 150 trap cycles, (f) vortex trajectory of vortex between 125 and 150 trap cycles showing that the vortex leaves the BEC after approximately 146 trap cycle in simulations 1 and 2. In simulations 3 and 4 we see that the vortex moves out only very slightly due to the very much longer time scale of the decay of the vortex (of the order of 700 trap cycles) when $\epsilon = 0.1$. All positions are in units of the harmonic oscillator length $r_0$. 
Figure 7.23: (Colour on-line) Breaking of axial symmetry for triangular vortex array showing (a) $z$-component of total angular momentum (upper black line) and condensate angular momentum (lower blue line) versus time, (b) change in thermal population $N_t(t) - N_t(0)$ versus time, and (c) change in condensate population $N_c(t) - N_c(0)$ versus time for (I) eccentricity parameter $\epsilon=0.25$ and turn-on time of five trap cycles, (II) eccentricity parameter $\epsilon=0.25$ and turn-on time of twenty trap cycles (see simulated absorption image in figure 7.24), (III) eccentricity parameter $\epsilon=0.1$ and turn-on time of five trap cycles, and (IV) eccentricity parameter $\epsilon=0.1$ and turn-on time of twenty trap cycles. The change in the populations $\Delta N_t$ and $\Delta N_c$ are given in units of the number of atoms $N$. All angular momenta are in units of $Nh$. 

Figure 7.24: Simulated absorption images [116] for breaking of axial symmetry for triangular vortex array over twenty trap periods with lattice parameter $a = 1.65\sqrt{3}$ for eccentricity parameter $\epsilon = 0.25$ after (a) 2.5, (b) 5, (c) 7.5, (d) 10, (e) 12.5, (f) 15, (g) 17.5, (h) 20, (i) 22.5, (j) 25, (k) 27.5, (l) 30, (m) 32.5, (n) 35, (o) 37.5, (p) 40, (q) 42.5, (r) 45, (s) 47.5, and (t) 50 trap cycles. All positions are in units of the harmonic oscillator length $r_0$. 
Figure 7.25: Breaking of axial symmetry for triangular vortex array for (I) turn-on time of five trap cycles for eccentricity parameter $\epsilon=0.25$, (II) for turn-on time of twenty trap cycles for eccentricity parameter $\epsilon=0.25$ (see simulated absorption image in figure 7.24), (III) for turn-on time of five trap cycles for eccentricity parameter $\epsilon=0.1$, and (IV) for turn-on time of twenty trap cycles for eccentricity parameter $\epsilon=0.1$ showing (a) x-displacement of vortex 1, (b) y-displacement of vortex 1, (c) trajectory of vortex 1, (d) x-displacement of vortex 2, (e) y-displacement of vortex 2, (f) trajectory of vortex 2, and (g) x-displacement of vortex 3, (h) y-displacement of vortex 3, and (i) trajectory of vortex 3. All positions are in units of the harmonic oscillator length $r_0$. 

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in good agreement with the time-dependent value estimated using a least-squares method of a slowly-varying sinusoid to the vortex x-displacement versus time (see figure 7.25 for $x_{pos}$ versus $T$ and $y_{pos}$ versus $T$). We also see good agreement with the value of the precessional frequencies of a single vortex (after the other two vortices have left the condensate) indicated in figure 7.25 again estimated using a least-squares method of a slowly-varying sinusoid to the vortex x-displacement versus time, and the time-independent predictions given in figure 7.5(a). We note that the simulation absorption images in figures 7.24 and the vortex trajectory diagrams in 7.25 II which show the vortex decay for the case where the eccentricity $\epsilon = 0.25$ is introduced over 20 trap cycles are consistent, indicating a decay time of $\sim 24$ trap cycles for the first vortex, and a decay time of $\sim 38$ trap cycles for the second. This is also consistent with figure 7.23 II which shows sudden changes in thermal density at these times, and a steady decrease in $L_z$ with slight drops accompanying the decay of each vortex. We also note a sudden change in the thermal density after $\sim 30$ trap cycles. This accompanies the complex precessional motion of the third vortex at $\sim 30$ trap cycles as shown in figures 7.25 II(g),(h) due to the interaction between the vortices. The lifetimes of the vortices in the case of the triangular vortex for $\epsilon = 0.25$ varies considerably - the first vortex to leave the condensate has a lifetime of between $\sim 20$ and $\sim 25$ trap cycles, while the second has a lifetime varying between $\sim 25$ and $\sim 38$ depending on the scenario - see figures 7.23 I(a)-(c) and 7.23 II(a)-(c). In all cases the loss of a vortex is characterised by a slight drop in $L_z$ and sudden increases in the thermal population with a corresponding drop in the condensate population (see figure 7.23). The departure of the vortices is also marked by the trajectories of the vortices shown in figures 7.25 I(a)-(f) and 7.25 II(a)-(f) where we see the end of the vortex tracks. The lifetime of the remaining vortex can only be inferred from figures 7.23 I(a) and 7.23 II(a) by extrapolation, and is of the order of 300-400 trap cycles (since the residual angular momentum (i.e. the angular momentum at the time that only a single vortex remains) is higher than in the single vortex case). In the case of the triangular vortex array for $\epsilon = 0.1$, the lifetime of the first vortex is of the same order ($\sim 25 \rightarrow 30$ trap cycles), but the lifetimes for the second and third vortices are considerably longer, the second vortex having an extrapolated lifetime of $\sim 400$ trap cycles (see figures 7.23 III and 7.23 IV). It is impossible to ascertain the lifetime of the remaining vortex from the simulations, but it is probably of the order of a few thousand trap cycles which is impractical to simulate with the facilities available.
7.6 Conclusions

By solving the orthogonal HFB equations in the frame rotating at the precessional frequency of the vortex predicted using the continuity equation for the condensate, and solving this self-consistently with the orthogonal HFB equations, we were able to predict the precessional frequency of off-axis vortices in BECs for given values of $a$ (the distance of the vortex from the axis) and $T$ (the temperature of the BEC). In these calculations, the vortex position is specified in the modified basis functions for the condensate wave-function. The precessional frequencies and LCLS energies for on-axis vortices were determined by extrapolation, and the LCLS energies found to be consistent with on-axis solutions to the orthogonal HFB equations for BECs having a single vortex rotating at the extrapolated precessional frequency. In this way we were able to demonstrate that there is no correlation between the LCLS energies and the precessional frequencies of off-axis vortices (contrary to that which was previously believed). We also established a correspondence between this formulation and a generalised multi-state model. These results are consistent with GPE simulations, and are also in qualitative agreement with the projected GPE simulations. We were able to generalise this technique to vortex arrays, and thus were able to produce plots of the precessional frequencies of these vortex arrays as a function of lattice parameter $a$ and temperature $T$. We also obtained qualitative agreement with the areal density approximation for the hexagonal vortex array.

These predictions were verified using time-dependent simulations in both the cases of the single off-axis vortex and of vortex arrays consisting of two, three and seven vortices. Simulations of a BEC stirred with one or three narrow-beam Gaussian stirrers also produced vortices precessing at frequencies in agreement with these predictions. In these simulations a critical stirring frequency about 10-20% in excess of the local Landau critical velocity for the creation of vortices within the Thomas-Fermi radius was found, and this is consistent with the notion already expressed that the critical velocity is increased by the presence of the energy gap in the HFB spectrum, and the fact that the HFB spectrum is steepened with respect to the Bogoliubov spectrum by the presence of the anomalous density. Finally we showed that breaking the axial symmetry of the trapping potential leads to loss of angular momentum of the BEC, and hence to vortex decay. We demonstrated this for both off-axis vortices, and for triangular vortex arrays by the introduction of an eccentricity $\epsilon$ into the trapping potential, and were able to establish approximate life-times for the vortices in both cases for $\epsilon = 0.25$, and $\epsilon = 0.1$. 
Chapter 8

Finite Temperature Mean Field Theory for 1D Optical Lattice

8.1 Introduction

Ultracold atoms confined within optical potentials [126] are of great current interest, both theoretically [127–140] and experimentally [141,142]. Optical lattices can be generated with extraordinary levels of control and used to simulate more complicated, less perfect and, often, less manipulable condensed-matter systems [143–146]. Ultracold atoms in optical lattices have also been proposed as candidates for quantum information processing [147], with applications in quantum cryptography and quantum computing. Various methods of loading and manipulating Bose-Einstein condensates in optical lattices have been proposed [148–152] and this is now routinely performed.

We consider a quasi-one-dimensional gas with tight radial confinement such that only axial degrees of freedom are available, but where the scattering is still effectively three-dimensional [153,154]. We then impose a one-dimensional optical lattice in the axial direction. We extend previous treatments at zero temperature [128,129] to finite temperature using the Hartree-Fock-Bogoliubov mean-field treatment as applied to a discrete Bose-Hubbard model, yielding modified Gross-Pitaevskii and Bogoliubov de Gennes equations. This set of equations is solved for both the case of a translationally invariant lattice (no external trapping potential) and an inhomogeneous lattice (optical lattice in an external harmonic trapping potential). The use of the mean-field based treatment means we can only consider the superfluid phase for the atoms in the optical lattice. The model is not
valid in the Mott insulator regime. We use the model to estimate the superfluid to normal phase-transition temperature in each case. We are then able to obtain a phase diagram for the superfluid and normal gas states in the low effective interaction strength limit. We note that Kleinert et. al. [155] have considered a homogeneous three-dimensional optical lattice (untrapped case) and predict an upward shift in the critical temperature which reduces once more for large effective interaction strengths to give re-entrant-type behaviour\(^1\). This is consistent with our findings for the one-dimensional system.

### 8.2 The Hartree-Fock Bogoliubov Treatment of a Bose Einstein Condensate in a one-dimensional Optical Lattice in the Popov Approximation

Let us consider a one-dimensional optical lattice with \(I\) lattice sites. If one expands the Bose field operators in the Wannier basis and applies the tight-binding approximation, one obtains the Bose-Hubbard model. The Bose-Hubbard Hamiltonian for atoms in a one-dimensional optical lattice may be written in the form [127–129]

\[
\hat{H} = \sum_{i=1}^{I} \hat{n}_i \epsilon_i - J \sum_{i=1}^{I} \left( \hat{a}^\dagger_{i+1} \hat{a}_i + \hat{a}^\dagger_i \hat{a}_{i+1} \right) + \frac{V}{2} \sum_{i=1}^{I} \hat{n}_i (\hat{n}_i - 1)
\]

(8.1)

where \(J\) represents the coupling strength between adjacent lattice sites, \(V\) is the interaction potential acting between atoms on the same site, and \(\hat{a}_i\) is the Bose field operator for the \(i^{th}\) lattice site, and \(\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i\). \(\epsilon_i\) is the non-interacting energy of the atoms on each site \(i\).

The usual commutation relations apply for the Bose field operator \(\hat{a}_i\), i.e.

\[
\left[ \hat{a}_j, \hat{a}_k^\dagger \right] = \delta_{j,k} , \quad [\hat{a}_j, \hat{a}_k] = [\hat{a}_j^\dagger, \hat{a}_k^\dagger] = 0.
\]

(8.2)

Assuming a macroscopic occupation of the ground state, we express the Bose annihilation operator for each lattice site \(i\) in terms of a complex part \(z_i\) and a fluctuation operator part \(\hat{\delta}_i\) as follows [128, 129]:

\[
\hat{a}_i = (z_i + \hat{\delta}_i) \exp \left( -\frac{i\mu t}{\hbar} \right).
\]

(8.3)

\(^1\)The phase diagram in figure 1 [155] (effective scattering length \(a_{eff}/a_c^{(0)}\) versus the temperature \(T/T_c^{(0)}\)) exhibits a re-entrant transition above the critical temperature \(T_c^{(0)}\) of the free system, i.e. the transition curve has a nose. This implies that for \(T > T_c^{(0)}\) it is possible to create a condensate by increasing \(a_{eff}\) which then disappears when \(a_{eff}\) is increased further.
We substitute equation (8.3) into the Hamiltonian (8.1) and take the self-consistent mean-field approximation such that \( \hat{\delta}_i \hat{\delta}_i \rightarrow \sum_i u_i^q \delta_i e^{-i\omega_q t} - v_i^q \delta_i^\dagger e^{i\omega_q t} \) (8.4)

with Hermitian conjugate

\[ \hat{\delta}_i^\dagger = \sum_q \left[ u_i^q \delta_i^\dagger e^{i\omega_q t} - v_i^q \delta_i e^{-i\omega_q t} \right] \] (8.5)

where \( u_i^q \) and \( v_i^q \) are the quasiparticle amplitudes, \( \omega_q \) are the quasiparticle excitation frequencies, \( \delta_i \) is the quasiparticle creator operator, and \( \delta_i^\dagger \) is the quasiparticle destructor operator.

Finally one obtains (for details see [128, 129]) the set of coupled equations (in dimensionless form) comprising the modified Gross-Pitaevskii equation

\[ \mu' z_i = \epsilon_i' z_i - (z_{i+1} + z_{i-1}) + V_{\text{eff}} (n_{ci} z_i + 2\tilde{n}_i z_i) \] (8.6)

and the Bogoliubov-de Gennes equations

\[ \epsilon_i' u_i^q + \epsilon_i^q z_i = [2V_{\text{eff}} (n_{ci} + \tilde{n}_i) - \mu' + \epsilon_i] u_i^q - [u_{i+1}^q + u_{i-1}^q] - V_{\text{eff}} z_i^2 u_i^q \]

\[ -\epsilon_i' v_i^q - \epsilon_i^q z_i = [2V_{\text{eff}} (n_{ci} + \tilde{n}_i) - \mu' + \epsilon_i] v_i^q - [v_{i+1}^q + v_{i-1}^q] - V_{\text{eff}} z_i^2 v_i^q \] (8.7)

with

\[ \tilde{n}_i = \langle \delta_i^\dagger \delta_i \rangle = \sum_q \left[ |u_i^q|^2 + |v_i^q|^2 + \left| \epsilon_i' \right|^2 \right] N_{\text{BE}} \left( \epsilon' \right) \] (8.8)

where

\[ N_{\text{BE}} \left( \epsilon' \right) = \frac{1}{Z^{-1} e^{\beta \epsilon'} - 1} \] (8.9)

is the usual Bose distribution and \( V_{\text{eff}} = V/J \), \( \mu' = \mu/J \), \( \epsilon_i' = \epsilon_i/J \), \( J = \hbar^2/2ma^2 \), and where we have assumed without loss of generality the condensate amplitudes \( z_i \) to be real (which they are to an arbitrary phase constant). \( \mu \) is the energy.
eigenvalue for the modified Gross-Pitaevskii equation (and approximates the chemical potential closely for values of temperature well below the transition temperature), $c^q$ is the energy eigenvalue of the Bogoliubov-de Gennes equations, and $\epsilon_i$ is the value of the trapping potential at site $i$. The $c^q$’s are necessary in order to ensure the orthogonality of the condensate with the excited states \[23, 24, 156\] and are given by

$$c^q = \frac{V}{N_0} \sum |z_j|^2 \left( z_j^* u_j^q - z_j v_j^q \right). \quad (8.10)$$

$Z$ is a fugacity term resulting from the difference between the true chemical potential $\mu_T$, and the chemical potential as estimated using the eigenvalue $\mu$ corresponding to the ground state of the modified Gross-Pitaevskii equation (equation (8.6)). Thus

$$Z = \exp \left( \beta (\mu_T - \mu) \right) \quad (8.11)$$

where $\beta = 1/k_B T$ is the temperature parameter, with $k_B$ Boltzmann’s constant and $T$ the temperature. Equation (8.8) follows in view of the fact that $\langle \hat{a}_q \hat{a}_{q'} \rangle = \langle \hat{a}_q^\dagger \hat{a}_{q'}^\dagger \rangle = 0$ and $\langle \hat{a}_q^\dagger \hat{a}_{q'} \rangle = N_{BE}(\epsilon_q) \delta_{qq'}$.

In the case of a homogeneous gas having a large number of particles in the ground state (ie. $n_c \gg 1$), the fugacity may be approximated by \[23, 24\]

$$Z = 1 + 1/n_c. \quad (8.12)$$

In these calculations we neglect these finite-size effects, which are only significant near the transition temperature $T_c$ and take the fugacity $Z$ to be unity.

We also require that the total number of atoms satisfy the condition \[129\]

$$N = \sum_{i=1}^I \left[ n_{c_i} + \tilde{n}_i \right] = \sum_{i=1}^I \left[ |z_i|^2 + \tilde{n}_i \right] = n_c + \tilde{n}. \quad (8.13)$$

The condensate fraction is simply

$$f_c = \frac{n_c}{n_c + \tilde{n}} = \frac{n_c}{N} = \frac{\sum_{i=1}^I n_{c_i}}{N} = \frac{\sum_{i=1}^I |z_i|^2}{N}. \quad (8.14)$$

Superfluid flow of the condensate occurs when there is a phase gradient. A phase gradient of the condensate modifies the hopping term of the Hamiltonian by the introduction of Peierls phase factors $e^{\pm i \Delta \phi}$ where $\Delta \phi$ is the phase factor between $\hat{a}_i$ and $\hat{a}_{i+1}$. The resulting energy shift may be estimated using second order perturbation theory. Since this energy shift is due entirely to the kinetic energy associated with the superfluid flow, and hence due to the
superfluid fraction, it follows that the superfluid fraction $f_s$ may be calculated in terms of this energy shift. It turns out that [128,129]

$$f_s = \frac{1}{N} \frac{E_\phi - E_0}{J (\Delta \phi)^2} = -\frac{1}{2N J} \langle \psi_0 | \hat{T} | \psi_0 \rangle - \frac{1}{N J} \sum_{\nu \neq 0} \left| \frac{\langle \psi_\nu | \hat{J} | \psi_\nu \rangle}{E_\nu - E_0} \right|^2 = f_s^{(1)} - f_s^{(2)}$$

(8.15)

where we have defined the operators

$$\hat{J} \equiv iJ \sum_{i=1}^I \left( \hat{a}_{i+1}^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_{i+1} \right)$$

and

$$\hat{T} \equiv J \sum_{i=1}^I \left( \hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{a}_{i+1} \right),$$

and where $E_0$ and $E_\nu$ are the energies corresponding respectively to the ground state $|\psi_0\rangle$ and the excited state $|\psi_\nu\rangle$, $\nu = 1, 2, ...$. Finally, we obtain the following expression for the superfluid fraction $f_S$ in terms of the condensate and quasiparticle amplitudes [128,129]:

$$f_s = f_s^{(1)} - f_s^{(2)}$$

(8.16)

where

$$f_s^{(1)} = \frac{1}{2N} \sum_{i=1}^I \left( \bar{z}_{i+1} z_i^* + z_{i+1}^* \bar{z}_i \right) + \sum_q \left( v_{i+1}^q v_i^{q*} + v_i^q v_{i+1}^{q*} \right)$$

(8.17)

and

$$f_s^{(2)} = \frac{J}{N} \sum_{q,q'} \left[ \frac{\left| \sum_i \left( u_{i+1}^q v_i^{q'} - u_i^q v_{i+1}^{q'} \right) \right|^2}{\hbar \omega_q + \hbar \omega_{q'}} + \delta_{qq'} \frac{\left| \sum_i \left( u_{i+1}^q v_i^{q'} - u_i^q v_{i+1}^{q'} \right) \right|^2}{2\hbar \omega_q} \right].$$

(8.18)

### 8.3 Translationally Invariant Lattice

In the case of a translationally invariant lattice, periodic boundary conditions apply, and the quasi-particle amplitudes are given by

$$u_j^q = \frac{u_j^q e^{i(qa)}}{\sqrt{I}}, \quad v_j^q = \frac{v_j^q e^{i(qa)}}{\sqrt{I}}, \quad 1 \leq j \leq I - 1.$$

(8.19)

Furthermore the condensate amplitudes are equal for each site $j$, thus $z_j = z$, $n_c = |z|^2 = z^2 = n_c$ for $1 \leq j \leq I - 1$ since $z$ has been taken without loss of generality to be real. Since there is no trapping potential, $\epsilon_i = \epsilon = 0$ for $1 \leq j \leq I - 1$. For the translationally invariant lattice

$$\mu = \left( \frac{|z|^2}{I} + 2n_c \right) V - 2J$$

(8.20)
where
\[ \tilde{n} = \frac{1}{I} \sum_q \left[ \|v^q\|^2 + (\|u^q\|^2 + \|v^q\|^2) N_{BE}(\epsilon^q) \right] \tag{8.21} \]
is the thermal population. Noting that \( \epsilon^q = 0 \) for the case of a translationally invariant lattice, it can be shown that for the translationally invariant lattice [129]

\[ \|u^q\|^2 = \frac{V z^2 + 4 J \sin^2 \left( \frac{q \pi}{2I} \right) + \hbar \omega_q}{2 \hbar \omega_q}, \tag{8.22} \]

\[ \|v^q\|^2 = \frac{V z^2 + 4 J \sin^2 \left( \frac{q \pi}{2I} \right) - \hbar \omega_q}{2 \hbar \omega_q}, \tag{8.23} \]

and

\[ \epsilon^q = \hbar \omega_q = \sqrt{K(q) [2 n_c V + K(q)]}, \tag{8.24} \]

where

\[ K(q) = 4 J \sin^2 \left( \frac{q \pi}{2I} \right). \tag{8.25} \]

Thus from equations (8.16), (8.17) and (8.18), for the translationally invariant lattice, the superfluid fraction is given by

\[ f_s = \frac{1}{N} \left( I \|z\|^2 + \sum_{j=1}^{I-1} \|v^q\|^2 \cos \left( \frac{2 \pi j}{I} \right) \right) \tag{8.26} \]
since \( q = 2 \pi j / I a \) for \( 1 \leq j \leq I - 1 \).

The condensate fraction for a given lattice site is given by \( f_c = n_c / n_0 \) where \( n_0 = N/I \) is the number of atoms per site. By equations (8.13) and (8.14), we have for the translationally invariant lattice,

\[ N = I \|z\|^2 + \tilde{n} = I \|z\|^2 + \sum_{j=1}^{I-1} \left[ \|v^{(j)}\|^2 + \left( \|u^{(j)}\|^2 + \|v^{(j)}\|^2 \right) N_{BE}(\epsilon^{(j)}) \right]. \tag{8.27} \]

To calculate the condensate and superfluid fraction for the translationally invariant lattice, we first determine the condensate amplitude. Then writing

\[ g_{j(n)} = \|z\|^2_{(n-1)} V_{eff} + 4 \sin^2 \left( \frac{\pi j}{I} \right), \tag{8.28} \]

\[ e_{j(n)} = 2 \sin \left( \frac{\pi j}{I} \right) \sqrt{2 \|z\|^2_{(n-1)} V_{eff} + 4 \sin^2 \left( \frac{\pi j}{I} \right)} \tag{8.29} \]

and

\[ N_{BE_{j(n)}} = \frac{1}{\exp \left( \beta e_{j(n-1)} \right) - 1} \tag{8.30} \]
where \( \beta' = J / \beta = J / k_B T = 1 / k_{\text{eff}} T \), with \( k_{\text{eff}} = k_B / J \), and where the subscript \((n)\) refers to the variable in question at the \(n\)th iteration, one can solve for \( |z|^2 \) using the iterative scheme

\[
|z|_n^2 = \frac{1}{N} \left( N - \sum_{j=1}^{I-1} \left( \frac{g_{j(n)} - e_{j(n)}}{2e_{j(n)}} + \frac{g_{j(n)} + e_{j(n)}}{2e_{j(n)}} N_{BE_{j(n)}} \right) \right).
\] (8.31)

As an initial guess, the value \( |z|_1^2 = \frac{N}{T} \) is used, and the calculations (8.28), (8.29), (8.30) and (8.31) repeated until convergence is attained (ie. \( |z|_n^2 - |z|_{n-1}^2 < \text{Error Tolerance} \)), or the maximum number of iterations is exceeded (divergent solution).

One first calculates \( g_{j(n)} \), \( e_{j(n)} \) and \( N_{BE_{j(n)}} \) using equations (8.28), (8.29) and (8.30). The quasiparticle amplitudes (given by equations (8.19)) may be calculated using the equations

\[
|u_{(j)}|^2 = \frac{g_{j(n)} + e_{j(n)}}{2e_{j(n)}} \] (8.32)

and

\[
|v_{(j)}|^2 = \frac{g_{j(n)} - e_{j(n)}}{2e_{j(n)}}. \] (8.33)

The condensate and superfluid fractions are then readily determined.

### 8.4 Inhomogeneous Lattice

The condensate amplitudes \( z_i \) are found by solving equation (8.6) where the trapping potential is given by \( \epsilon_i = \Omega \left[ i - (I + 1)/2 \right]^2 \) for site \( i \) with \( \Omega = \frac{1}{2m} \omega^2 a^2 \), and \( a \) is the inter-lattice spacing. The quasi-particle amplitudes for site \( i \), \( u_i^q \) and \( v_i^q \) are found by solving equations (8.7).

This set of equations can again be solved iteratively. In performing this calculation, we actually set the \( c^q \)'s to zero when solving the Bogoliubov-de Gennes equations, but do so in the GGPE basis, thus ensuring orthogonality of the ground state and the excited states [23, 24]. The GGPE basis is given by the normalised solutions to the eigenvalue problem given by equation (8.6), with the ground state (zero energy solution) excluded.

Let us rewrite the Bogoliubov-de Gennes equations (8.7) in matrix form

\[
\epsilon^q \begin{bmatrix} u^q \\ v^q \end{bmatrix} = \begin{bmatrix} \hat{\mathcal{L}} & M \\ -M & -\hat{\mathcal{L}} \end{bmatrix} \begin{bmatrix} u^q \\ v^q \end{bmatrix} \] (8.34)
where

$$u^q = \begin{bmatrix} u^q_{q-I} \\ \vdots \\ u^q_i \\ \vdots \end{bmatrix}, \quad v^q = \begin{bmatrix} v^q_{q-I} \\ \vdots \\ v^q_i \end{bmatrix}$$

(8.35)

$$\hat{L} = 2V_{\text{eff}} (n_{ci} + \bar{n}_i) - \mu + \Omega i^2 - \hat{J}$$

(8.36)

and

$$M = -V_{\text{eff}} z_i^2.$$  

(8.37)

Here $\hat{J}$ is defined as the operator acting on $z_i$, $u^q_i$, and $v^q_i$ as follows:

$$\hat{J} u^q_i = u^q_{i+1} + u^q_{i-1}$$

(8.38)

for example. In deriving equation (8.6), we used the fact that we can take the condensate amplitudes $z_i$ (without loss of generality) to be real.

Now, let $\{z_i^q\}$ constitute the eigenstates of equation (8.6) with eigenvalues $\mu^q$. We order the normalised eigenvalues into ascending order, and order the eigenstates accordingly, call these $\{\xi_i^q\}$. The state $\xi_i^0$ corresponds to the Goldstone mode, we must exclude this in order to obtain the GGPE basis. Let us define the matrix

$$\mathbf{U} = \begin{bmatrix} \xi^1 & \ldots & \xi^q & \ldots & \xi^{2l} \end{bmatrix}$$

(8.39)

where

$$\xi^q = \begin{bmatrix} \xi_i^q \\ \vdots \\ \xi_i^q \\ \vdots \end{bmatrix}. \quad (8.40)$$

Let $\{u^q_{HF B}, v^q_{HF B}\}$ be the solution to the Bogoliubov-de Gennes equations in the GGPE basis, then the solution to the matrix equation

$$\epsilon^q \begin{bmatrix} u^q_{HF B} \\ v^q_{HF B} \end{bmatrix} = \begin{bmatrix} U^T \hat{L} U & U^T M U \\ -U^T M U & -U^T \hat{L} U \end{bmatrix} \begin{bmatrix} u^q_{HF B} \\ v^q_{HF B} \end{bmatrix}$$

(8.41)

gives the Bogoliubov quasiparticle amplitudes in the GGPE basis. To obtain the Bogoliubov quasiparticle amplitudes $\{u^q_i, v^q_i\}$ one transforms back using

$$u^q = U u^q_{HF B}, \quad v^q = U v^q_{HF B}. \quad (8.42)$$
The numerical procedure for the problem is then as follows:

1. Solve the dimensionless modified Gross-Pitaevskii equation, equation (8.6). Hence calculate the condensate population $n_{ci}$ for each lattice site $i$ using $n_{ci} = |z_i|^2$.

2. Determine the GGPE basis by solving the eigenvalue problem given by equation (8.6), ordering the eigenvalues and hence the eigenvectors accordingly, and then eliminating the Goldstone mode, checking that this is indeed proportional to the ground state as calculated in step 1.

3. Solve the Bogoliubov-de Gennes equations in the GGPE basis by solving the eigenvalue problem given by equation (8.41), ordering the eigenvalues and eliminating the negative energy eigenstates and the zero energy eigenstate, and hence obtain the quasiparticle amplitudes $\{u^q_i, v^q_i\}$ by applying the transformation given by equation (8.42).

4. Calculate the quasiparticle population $\tilde{n}_i$ for each lattice site $i$ using equation (8.8).

5. Repeat steps 1, 2, 3 and 4 until the convergence condition is satisfied.

6. Hence calculate the condensate fraction and the superfluid fraction using equations (8.14), (8.16), (8.17) and (8.18).

\section{8.5 Results}

We present results for various effective interaction strengths consistent with the parameters defined in reference [156] and using the band structure calculations of [157].

\subsection*{8.5.1 Results for the Case of the Translationally Invariant Lattice}

In Figures 8.1 and 8.2 we present results for a translationally invariant lattice with one atom and ten atoms per site, respectively, for various values of the effective interaction potential $V_{eff}$. In both cases ten lattice sites, with periodic boundary conditions, were used. One observes a decrease in both the condensate and superfluid fractions with temperature\footnote{The dotted lines shown in figures 8.1 (a),(b) and 8.2 (a) indicate where the plots of the overall condensate/superfluid fractions versus temperature for the three interaction strengths become unreliable, but are included for completeness.}, and
Figure 8.1: Translationally invariant lattice with ten atoms and ten sites (i.e., one atom per lattice site). Overall condensate (a) and superfluid (b) fractions as a function of temperature for effective interaction strengths of 0.001 (dashed line), 1 (dot-dashed line), and 20 (solid line). The corresponding phase diagram is shown in panel (c). “S” represents the superfluid phase, and “N” the normal phase, and the circles the critical temperature corresponding to the respective interaction strength.
Figure 8.2: Translationally invariant lattice with ten atoms per site showing (a) condensate fraction for effective interaction strengths of 0.001 (dashed line), 0.1 (dot-dashed line), and 50 (solid line), (b) excitation spectrum as a function of temperature for effective interaction strength of 50, and (c) the corresponding phase diagram. “S” represents the superfluid phase, and “N” the normal phase, and the circles the critical temperature corresponding to the respective interaction strength.
we interpret the point at which these densities approach zero as indicative of the critical temperature $T_c$ for the superfluid to normal gas phase transition. Our calculations make the assumption that the true chemical potential and the lowest energy eigenvalue for the modified Gross-Pitaevskii equation are equal. This tends to underestimate the transition temperature$^3$, but should provide a useful criterion for the transition between superfluid and normal behaviour$^4$. This interpretation is supported by an examination of the low-lying excitation spectrum$^5$ which, for the case $V_{eff} = 50$, is shown in panel (b) of figure 8.2. The “softening” of the modes, indicative of the phase transition, is clearly seen and coincides with the transition temperature obtained by noting the temperature at which the condensate and superfluid densities approach zero.

We obtain such a “transition”$^6$ temperature for each value of the effective interaction potential $V_{eff}$, producing a phase diagram as shown in figures 8.1(c) and 8.2(c), where the superfluid phase and the normal phase are as indicated, the superfluid phase lying to the left of the curve. The transition to the Mott insulator phase cannot be accounted for by this formalism, but would in practice occur when $V_{eff} = V/J$ exceeds some critical value. In all instances, the critical temperature for the transition from superfluid to normal gas increases with the effective interaction potential, as is indeed the case with a homogeneous Bose gas (i.e. a Bose gas in the absence of an optical lattice and confining potential) [158,159]. This behaviour has also been predicted by Kleinert et. al [155]. Our results are consistent with their conclusions. In addition, they predict a reduction of the critical temperature as the effective interaction strength is increased further. We, however, are unable to explore this regime for the one-dimensional lattice as it extends beyond the validity of our model.

### 8.5.2 Results for the Case of the Inhomogeneous Lattice

Figure 8.3 shows plots of the number of condensate atoms, excited atoms and of the total number of atoms for each lattice site for the case of an inhomogeneous optical lattice

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3For an infinite, homogeneous one-dimensional lattice (no external trapping potential), the transition temperature is zero, so no superfluid behaviour is ever possible. Here we are interested in the shift in critical temperature due to the effect of interactions which we obtain by considering a finite system.

4Note that, in the Bose-Hubbard model, the condensate number approaches the filling factor as the temperature tends to infinity, so the condensate and superfluid fractions are never strictly zero for the finite size system.

5The lines shown in figure 8.2 (b) represent the quasi-particle excitation energies $q = 0, 1, 2, 3$ in ascending order.

6We only see a “transition” because of the finite size of our system. There is, however, no transition in the thermodynamic limit.
Figure 8.3: Inhomogeneous lattice with 41 lattice sites and ten atoms in total for $V_{\text{eff}} = 0.5$, at (a) $T = 0\text{nK}$, (b) $T = 1\text{nK}$ (c) $T = 1.6\text{nK}$. Circles represent the number of condensate atoms, squares represent the number of excited atoms and crosses the total number of atoms.
Figure 8.4: Overall condensate and superfluid fractions as a function of temperature, and the corresponding phase diagram for an optical lattice in a harmonic potential with 40 lattice sites (even case) and ten atoms. (a) corresponds to the condensate fraction, (b) to the superfluid fraction for effective interaction strengths of 0.001 (dashed line), 0.5 (dot-dashed line), and 2 (solid line), and (c) to the phase diagram. “S” represents the superfluid phase, and “N” the normal phase.
consisting of 41 lattice sites (odd case) with ten atoms in total. The plots are for $V_{\text{eff}} = 1$ at various temperatures ranging from $T = 0$ to $T = 1.6\text{nK}$. At zero temperature, the condensate atom distribution is bell-shaped, peaked at the central lattice site. There is a small quantum depletion even at zero temperature, and the distribution of excited atoms is shaped as a bimodal distribution, centred about the central lattice site. As the temperature increases, the condensate population decreases, but the distribution still remains bell-shaped, and the excited population increases. In figure 8.4 we present the overall condensate and superfluid fractions and the corresponding phase diagram for optical lattices in a harmonic potential consisting of 40 lattice sites (even case). Panel (a) corresponds to the condensate fraction, (b) the superfluid fraction, and (c) the phase diagram. The dotted lines shown in panels (a) and (b) indicate where the plots of the overall condensate and superfluid fractions versus temperature for the three interaction strengths become unreliable, but are included for completeness. We note that for higher temperatures, calculations performed using 41 lattice sites begin to show a marked difference. This is indicative of the fact that we are pushing the bounds of validity of our model. In particular we are seeing significant finite size effects, which affect the value of the chemical potential and, ultimately, a failure of the mean field approximation. The dotted continuation of the lines in figure 8.4 indicate where our calculations become unreliable, but are included for completeness. We are still able to use our model to obtain an estimate of the critical temperature and hence the trend in its dependence upon the effective interaction strength, using the same criterion as for the homogeneous case. We therefore conclude from figure 8.4 that the superfluid to normal phase transition temperature increases with increasing $V_{\text{eff}}$. It is clear, then, that the shift in critical temperature with effective interaction potential is positive definite for a Bose gas in a one-dimensional optical lattice, regardless of whether the system is confined in a (harmonic) trapping potential or not. This is in contrast to the case of a three-dimensional Bose gas without the optical lattice, where $\Delta T_c$ changes sign for the trapped gas.

As before, we can say nothing about the Mott insulator region, except that one would expect the Mott insulator phase for small inter-site coupling strength $J$ (and hence large $V_{\text{eff}}$).
8.6 Conclusions

We have applied the discretized Hartree-Fock-Bogoliubov formulation to the Bose-Hubbard model in order to calculate the dependence of the condensate and superfluid fractions on the temperature. We have used this to estimate the critical temperature for the superfluid to normal phase transition for both a translationally invariant optical lattice (no external trap present), and an inhomogeneous optical lattice (contained within an external harmonic trap). This has enabled us to investigate the phase diagram for both cases and we observe that the transition temperature increases with increasing effective interaction potential $V_{eff}$. Unlike the homogeneous case with no optical lattice, this positive shift in the critical temperature with interaction strength is present in both the translationally invariant case and when a harmonic confining potential is imposed. In the homogeneous gas the shift in the critical temperature is only positive in the absence of a confining potential. These conclusions are consistent with previous work for the translationally invariant case [155] in three dimensions, extending this result to include harmonic confinement.
Chapter 9

Conclusions

9.1 Background

In this thesis we developed an orthogonalised HFB theory which we applied to BECs vortices in harmonically confined BECs. In chapter 2 we reviewed the theoretical background for such a treatment, and commenced with the equivalence between the first and second quantised representations of the quantum many-body problem. We then investigated various approaches in solving the many-body problem in the second quantised form, focussing mainly on number-conserving and symmetry-breaking mean-field theories. Since coherent states do not have well-defined number eigenstates, symmetry-breaking mean-field formalisms violate number conservation, but introducing a chemical potential as a Lagrange multiplier, and working in the Grand-Canonical ensemble ensures that particle number is conserved. In the symmetry-breaking approach the Bose field operator is split into a c-field part representing the condensate, and a fluctuation operator part. To lowest order, neglecting the thermal part yields the Gross-Pitaevskii Equation (GPE) which is a $T = 0$ theory. If we excite the condensate and retain perturbation terms to lowest order, we can calculate the collective excitations of the condensate (linear response theory), and these equations correspond to the Bogoliubov-de Gennes equations (BdGEs) in the Bogoliubov approximation. In deriving the BdGEs we transformed the thermal part (the fluctuation operator) into a basis of non-interacting quasi-particles representing the elementary excitations, and this is justified with its correspondence at $T = 0$ (Bogoliubov approximation) with the linear response theory. At finite temperature we obtain the Hartree-Fock-Bogoliubov (HFB) equations which suffer from various theoretical problems, not least of which is the unphysical gap in the quasi-particle spectrum and the violation of Hugenholtz-Pines The-
orem [11]. We considered various approximations which exist in the literature, showing that these result in gapless theories which rectify this problem, but unfortunately these result in violation of important conservation laws. Other problems associated with the HFB formalism are the fact that the condensate and non-condensate quasi-particle amplitude wave-functions are not orthogonal, and the so-called Grand-Canonical catastrophe. We discussed these issues in chapter 2, and later in chapter 4, where we proposed an orthogonal formalism which ensures that the condensate and thermal populations are always orthogonal, thereby also ensuring the existence of a zero-energy excitation. We also considered briefly in chapter 2, two other approaches, namely, the projected Gross-Pitaevskii and the truncated Wigner approaches.

In chapter 3 we presented a brief survey on topological defects in BECs. Topological defects occur as a result of phase-discontinuities in the BEC, examples of which are vortices, which have a phase circulation about the point of zero density with a corresponding phase discontinuity of a multiple of $2\pi$ - usually $2\pi$ because multiply-charged vortices are very unstable and soon break up into singly charged vortices.

Just to recap, the categories of formalisms considered here (which we presented in chapters 2 and 4) are:

1. Symmetry-breaking Mean-Field Theories, and
2. Number-conserving Mean-Field Theories

and may be summarised as follows\(^1\):

**Symmetry-breaking Mean-Field Theories**

1. The Gross-Pitaevskii Equation (GPE) [5–9] where the Bose field operator is regarded as a mean-field, and replaced by a c-number. We saw in chapter 2 that this represents the Hamiltonian to zeroth order, and yields the GPE. We saw further that the excitations can be found using linear response theory [6–10] yielding the Bogoliubov-de Gennes Equations (BdGEs) in the Bogoliubov approximation.

2. The Hartree-Fock-Bogoliubov (HFB) Formalism [11] where the Bose field operator is separated into a condensate and a thermal fluctuation operator. We used the

\(^1\)We also considered classical field theories and the truncated Wigner formalism, but these were dealt with only very briefly.
Bogoliubov transformation to de-compose the thermal fluctuation operator into a basis of non-interacting quasi-particles. We considered the condensate part to be a mean field, represented by a c-field, thus leading to the breaking of the $U(1)$ symmetry of the Hamiltonian, and hence to the violation of particle conservation. However, we saw in chapter 2 how this problem may be overcome by considering the Grand-Canonical Hamiltonian, where we introduced the chemical potential $\mu$ as a Lagrange multiplier, thereby ensuring particle conservation. This led to the HFB equations consisting of a generalised Gross-Pitaevskii equation (GGPE) for the condensate, and a set of BdGEs for the quasi-particle amplitudes. We noted that the HFB formalism is a conserving theory, i.e. the conservation laws are satisfied, but that the symmetry-breaking resulted in various problems, one of which is an unphysical gap in the quasi-particle energy spectrum, violating the Hugenholtz-Pines theorem [11], and the Grand-Canonical catastrophe [12, 13]. We pointed out that, in view of the approximations concerning the mean-field, HFB theory is valid for low temperatures, typically for $T \lesssim T_c/2$.

3. The Popov Approximation to the full HFB theory [11] where the energy gap problem is addressed by ignoring the anomalous density. The argument presented is that two-body correlations are represented by the anomalous density $\tilde{m}$, and therefore the s-wave scattering length $a_s$ is already measured in the presence of two-body collisions (correlations). In order to understand this we noted that the contact potential approximation $U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$ where $g$ is the interaction parameter given by $g = 4\pi\hbar^2a_s/m$ used here represents an approximation to the 2-body T-matrix, and not to the bare interaction potential $U(\mathbf{r} - \mathbf{r}')$. Using this approximation, one achieves a gapless quasi-particle energy spectrum. However, as we saw in chapter 4, the number and linear/angular momentum conservation laws are violated.

4. The G1 and G2 Gapless Theories [15, 19, 21] where one proceeds beyond the two-body T-matrix by replacing the contact potential approximation to the interaction potential in the GPE and in the BdGEs in the Bogoliubov approximation by the expression $g \left( 1 + \frac{\tilde{m}(\mathbf{r})}{\Phi^2(\mathbf{r},t)} \right)$ thereby introducing the anomalous density into the formalism. As in the case of the Popov approximation, one achieves a gapless quasi-particle energy spectrum. However, as we showed in chapter 4, the number and linear/angular momentum conservation laws are again violated.

5. The orthogonal HFB formalism presented in chapter 4 which, as we demonstrated in section 4.3.1, has a zero-energy excitation. We showed in sections 4.3.3-4.3.5 that the
physical conservation laws of particle, energy and angular momentum conservation are all satisfied.

**Number-conserving Mean-Field Theories**

1. The formalism proposed by C. W. Gardiner [22], which is a $T = 0$ theory, and essentially yields the GPE, where the excitations for quasi-particle modes may be determined using the BdGEs in the Bogoliubov approximation.

2. The formalism proposed by S. A. Morgan [23,24], which is a finite temperature theory using first order perturbation theory to take into account the quadratic terms in the thermal fluctuation operator, and second-order perturbation to determine the energy shifts due to the higher order terms. This yields a set of equations consisting of the GGPE (as in HFB theory), and a modified set of BdGEs where the Hamiltonian is no longer diagonalisable in terms of the quasi-particle energies (as is the case in HFB), but where there is dependency on the excitation energy in the BdGEs for each of the quasi-particle modes.

3. The formalism proposed by Y. Castin and R. Dum [25] where a number-conserving approach (together with an appropriate form for the fluctuation operator) is used to obtain a systematic expansion of the Hamiltonian. The dynamical equations are then derived for the condensate and the quasi-particle amplitudes to various orders. To first order, the GPE is recovered, with the quasi-particle amplitudes described by the BdGEs in the Bogoliubov approximation. Subsequent orders yield higher order corrections to these equations.

4. The formalism proposed by S. A. Gardiner and S. A. Morgan [26] where a number-conserving approach is used along similar lines to Y. Castin and R. Dum [25], but where they choose a slightly different fluctuation operator, again obtaining a systematic expansion of the Hamiltonian. The dynamical equations are then derived for the condensate and the quasi-particle amplitudes to various orders yielding a generalised form for the GPE, and a set of modified BdGEs. We discussed this formalism in more detail in chapter 2, together with some of the problems associated with this formalism.
9.2 Work done

9.2.1 Development of Orthogonal HFB and Computational Implementation

In Chapter 4 we developed further theory pertaining to the HFB formalism and introduced an orthogonal HFB formalism which allows for a zero-energy excitation, in contrast to the standard HFB formalism (see section 4.3.1). We showed in sections 4.3.3-4.3.5 that the physical conservation laws of particle, energy and angular momentum conservation are still satisfied, and presented in sections 4.3.8 perturbation calculations by which the quasi-particle spectrum might be corrected, thus yielding a gapless theory in which all important conservation laws are satisfied. In section 4.3.6 we derived an equation from the continuity equation for the condensate density predicting the precessional frequencies of off-axis vortices (including vortex arrays, provided the vortices are not too close), which we then solved self-consistently with the time-independent orthogonal HFB equations in the frame rotating at the vortex precessional frequency.

In chapter 5 on numerical methods, we explored methods by which the time-independent and time-dependent calculations may be performed, including the calculation of the precessional frequencies of vortices.

9.2.2 Evaporative Cooling 'Toy Simulations'

In chapter 6 we simulated the evaporative cooling of 2D BECs in axially-symmetric harmonic traps using time-dependent HFB theory, and used time-independent HFB theory to estimate the effective temperature at various times during the evaporative cooling process. We found that the system equilibrates to a reasonable approximation provided the cooling process is not too rapid. We found, however, no evidence of condensate growth, although cooling of the condensate is achieved. This is due to the fact that significant damping processes, the Landau and Beliaev processes are not accounted for in HFB due to the application of Wick’s theorem for ensemble averages. A dynamical thermal cloud is required to account for the Landau and Beliaev damping processes, and this is not the case in standard HFB and orthogonal HFB.
9.2.3 Vortex Dynamics in Quasi-2D BECs

In chapter 7 we investigated vortices in 2D BECs in axially-symmetric harmonic traps using the orthogonal HFB theory developed in chapter 4. In section 7.2 we found solutions for on-axis vortices, determining the energy spectrum and hence the lowest core localised state (LCLS) energies. We showed in section 7.3 that the precessional frequency for an off-axis vortex (or for several off-axis vortices) may be predicted using the continuity equation for the condensate, and solving self-consistently with the HFB equations in the rotating frame. We showed that these predicted precessional frequencies are consistent with the $T = 0$ case, and are entirely uncorrelated with the LCLS energies. We have seen that this method provides an efficient method for solving the off-axis vortex problem, and also works very well for vortex arrays, since the position of the vortices is incorporated into the modified basis functions defined in this thesis in sections 5.3.1, 7.4.1 and 7.4.2. We have also seen that the continuity equation for the condensate density predictions for the precessional frequency of single off-axis vortices and of vortex lattices is accurate and is in very good agreement with time-dependent simulations. In section 7.3.1 we created an off-axis vortex using the two-state model, and we see that this model is only valid for extremely weak interactions, and breaks down rapidly as we increase the interactions, becoming meaningless at the interaction strengths considered here (which are only moderate). In section 7.3.2 we generalised the two-state model to a generalised multi-state model and use the normalisation conditions for the model to derive an equation predicting the precessional frequency of the vortex. We showed the equivalence of the multi-state model with the method described in section 7.4.1 where we specified the position of the vortex using modified basis functions for the condensate wave-function and solved the HFB equations self-consistently in the frame rotating at the precessional frequency as predicted by the continuity equation for the condensate density. We found numerically (see figure 7.13) that there is excellent agreement between the two predictions provided the mode cut-off is sufficient. In section 7.4.3 we also calculated the precessional frequencies for two vortices, triangular vortex arrays, and hexagonal vortex arrays, and the precessional frequencies are compared in figure 7.12.

In section 7.5 we used the time-dependent HFB equations to create vortices by stirring the BEC by means of a Gaussian optical potential (section 7.5.2) and examined the conservation of angular momentum and how breaking the axial symmetry of the harmonic trapping potential leads to loss of angular momentum, and hence to the decay of vortices (section 7.5.3). We found in section 7.5.2 very good agreement of the measured preces-
sional frequencies of the vortices in stirred BECs with the predicted values in section 7.4.3. In section 7.5.2 we found the existence of a critical stirring frequency (corresponding to a velocity of the stirring potential through the fluid of just 10 – 20\% in excess of the Landau critical frequency), below which no vortices are created in regions of appreciable superfluid density (i.e. within the Thomas-Fermi radius). No experiments have been performed on stirring a BEC using a narrow rotating probe as considered here but experiments [42] have been performed which show evidence of a critical stirring angular velocity using elliptical deformation of the trap. Experiments to test the superfluid critical velocity using the linear motion of a narrow probe laser beam have also been performed [118–120], finding critical velocities for the onset of dissipation ∼ 5 – 10 times smaller than the critical velocity inferred from the bulk Bogoliubov speed of sound. Time-dependent GPE simulations [121] also indicate that dissipation first occurs at speeds significantly less than the speed of sound. However, the linear motion of the probe in these works excite vortex dipole or solitons, and are not therefore directly applicable to the present work.

In a previous study [90, 105], similar stirring simulations were carried out using time-dependent GPE simulations. However, the critical stirring frequency referred to in these results are the thermodynamic critical frequency (at which the vortex-free and central vortex states have equal energies), whereas the results presented here refer to the critical frequency at which vortices are created within the Thomas Fermi radius. Nevertheless, the results of [90, 105] are consistent with the simulations performed in this work.

### 9.2.4 1D Optical Lattices in the HFB Popov Approximation

In chapter 8 we applied finite temperature mean-field theory of BECs in 1D optical lattices using HFB mean-field theory in the Popov approximation. We calculated the superfluidity of the BEC in a 1D optical lattice in two situations:

1. No trapping potential (periodic boundary conditions),

2. In the presence of a harmonic trapping potential.

In both cases we extrapolated the superfluidity calculations as a function of temperature to estimate a superfluid-normal fluid transition temperature, thus obtaining phase diagrams for the homogeneous and inhomogeneous cases.
9.3 Further Work

Further work that could be undertaken along the lines of the work already done in this thesis could be:

1. Incorporating a damping term in the orthogonal HFB formalism such that the conservation laws are still satisfied. Such a term would approximate the scattering terms neglected in the mean-field formalism, and would lead to a growth term for the condensate which is not present in the formalism presented here. It is hoped by incorporating such a term to obtain condensate growth which is not seen in the BEC cooling simulations performed in chapter 6. There are several theories that would need to be investigated in this type of approach, for example the Zaremba-Nikuni-Griffin (ZNG) model [160], the work done by Walser Tet. al. [161, 162], and Proukakis [163]. The important issue here is that the conservation laws are satisfied.

2. Using orthogonal time-dependent HFB to simulate disorder due to speckle [164]. Disorder has also been produced experimentally by means of an incommensurate optical lattice [165], but the suggestion here would be to perform the 1D disorder calculations as in [167,168] at finite temperature. This could prove quite challenging in view of the large grid sizes, and the large number of grid points required.

3. Using three-dimensional orthogonal time-dependent HFB calculations to reproduce the results in the JILA experiment [20] was considered, but the calculations were considered to be numerically too costly for the computing facilities currently available. Numerical techniques employing discrete variable representation [166] as opposed to the spectral representation employed here could be used to substantially reduce the numerical effort in calculating the matrix elements, but it is unclear at present how practical these calculations will be. Another possibility for 3D HFB simulations would be the vortex calculations to investigate the effect of external perturbations (for example, noise), on the vortex lines at finite temperature.
Bibliography


Bibliography


[116] The simulated absorption images shown here are logarithmic plots given by \( n_{\text{plot}} = \log \left( \frac{n}{n_{\text{max}}} \right) \), where \( n \) refers to the relevant density to be plotted, and \( n_{\text{max}} \) is the overall maximum density of the BEC (i.e. the maximum of the sum of the condensate and non-condensate densities).

[117] It should be noted that in all cases the precessional frequency of the vortices nucleated in the stirring is distinct from the rotational frequency of the stirrer itself - see for example, figure 7.19 II which shows clearly that these precessional frequencies are uncorrelated with the stirring frequency \( \Omega_{\text{stir}} = 0.5\omega_r \).


Appendix A

Properties of the HFB and Orthogonal HFB Formalism

A.1 Standard HFB

A.1.1 Commutation Relations for Bose Field Operators

Let \( \hat{\psi}(\mathbf{r}, t) \) be a Bose field operator satisfying the usual Bose commutation relations

\[
\left[ \hat{\psi}(\mathbf{r}_1, t), \hat{\psi}^\dagger(\mathbf{r}_2, t) \right] = \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad \left[ \hat{\psi}(\mathbf{r}_1, t), \hat{\psi}(\mathbf{r}_2, t) \right] = 0, \quad \left[ \hat{\psi}^\dagger(\mathbf{r}_1, t), \hat{\psi}(\mathbf{r}_2, t) \right] = 0.
\] (A.1)

Suppose as in standard HFB that we follow the spontaneous symmetry-breaking approach writing

\[
\hat{\psi}(\mathbf{r}, t) = \Phi(\mathbf{r}, t) + \hat{\eta}(\mathbf{r}, t)
\] (A.2)

Since \( \Phi(\mathbf{r}, t) \) is a c-field, we find that the fluctuation operator \( \hat{\eta}(\mathbf{r}, t) \) also obeys the Bose commutation relations

\[
\left[ \hat{\eta}(\mathbf{r}_1, t), \hat{\eta}^\dagger(\mathbf{r}_2, t) \right] = \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad \left[ \hat{\eta}(\mathbf{r}_1, t), \hat{\eta}(\mathbf{r}_2, t) \right] = 0, \quad \left[ \hat{\eta}^\dagger(\mathbf{r}_1, t), \hat{\eta}^\dagger(\mathbf{r}_2, t) \right] = 0.
\] (A.3)

Suppose that we make the Bogoliubov transformation

\[
\hat{\eta}(\mathbf{r}, t) = \sum_k \left( u_k(\mathbf{r}, t) \hat{a}_k + v_k^*(\mathbf{r}, t) \hat{a}_k^\dagger \right)
\] (A.4)

with Hermitian conjugate

\[
\hat{\eta}^\dagger(\mathbf{r}, t) = \sum_k \left( v_k(\mathbf{r}, t) \hat{a}_k + u_k^*(\mathbf{r}, t) \hat{a}_k^\dagger \right)
\] (A.5)
Appendix A. Properties of the HFB and Orthogonal HFB Formalism

which we did in chapters 2 and 4 in order to transform into a non-interacting quasi-particle basis for the fluctuation operator \( \hat{\eta}(r,t) \). Since the Bogoliubov transformation is canonical, the quasi-particle creation and annihilation operators \( \hat{a}^\dagger_k \) and \( \hat{a}_k \) also satisfy the Bose commutation relations

\[
[\hat{a}_k, \hat{a}^\dagger_l] = \delta_{k,l} \quad \text{and} \quad [\hat{a}_k, \hat{a}_l] = [\hat{a}^\dagger_k, \hat{a}^\dagger_l] = 0 \quad (A.6)
\]

and hence we also have from (A.4) and (A.5) the commutation relations

\[
[\hat{\eta}(r,t), \hat{a}^\dagger_{q}] = u_q(r,t), \quad [\hat{\eta}_{q}(r,t), \hat{a}_l] = v^*_q(r,t), \quad [\hat{\eta}^\dagger(r,t), \hat{a}^\dagger_{q}] = v_q(r,t), \quad [\hat{\eta}_q(r,t), \hat{a}^\dagger_l] = u^*_q(r,t). \quad (A.7)
\]

Since \( \Phi(r,t) \) is a c-field, we deduce that

\[
[\hat{\psi}(r,t), \hat{a}^\dagger_{q}] = u_q(r,t), \quad [\hat{\psi}_q(r,t), \hat{a}_l] = v^*_q(r,t), \quad [\hat{\psi}^\dagger(r,t), \hat{a}^\dagger_{q}] = v_q(r,t), \quad [\hat{\psi}_q(r,t), \hat{a}^\dagger_l] = u^*_q(r,t). \quad (A.8)
\]

A.1.2 Symmetry and Orthogonality Properties of the Bogoliubov Transformation

Since the Bogoliubov transformation is canonical, and hence the commutation relations (A.6) hold, we have the following symmetry and orthogonality properties of the Bogoliubov transformation:

1. The normalisation condition

\[
\int d\mathbf{r} \left( u^*_k(\mathbf{r},t)u_l(\mathbf{r},t) - v^*_k(\mathbf{r},t)v_l(\mathbf{r},t) \right) = \delta_{k,l} \quad (A.9)
\]

for the quasi-particle amplitudes is satisfied,

2. The symmetry conditions

\[
\int d\mathbf{r} \left( u_k(\mathbf{r},t)v_l(\mathbf{r},t) - v_k(\mathbf{r},t)u_l(\mathbf{r},t) \right) = 0 \quad (A.10)
\]

and its complex conjugate

\[
\int d\mathbf{r} \left( u^*_k(\mathbf{r},t)v^*_l(\mathbf{r},t) - v^*_k(\mathbf{r},t)u^*_l(\mathbf{r},t) \right) = 0 \quad (A.11)
\]

holds.
Now
\[ \int d\mathbf{r} \left( u^*_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) - v^*_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) \right) = \sum_t \left[ \int d\mathbf{r} \left( u^*_k(\mathbf{r}, t) u_l(\mathbf{r}, t) - v^*_k(\mathbf{r}, t) v_l(\mathbf{r}, t) \right) \hat{a}_t \right. \\
+ \left. \int d\mathbf{r} \left( u^*_k(\mathbf{r}, t) v_l(\mathbf{r}, t) - v^*_k(\mathbf{r}, t) u_l(\mathbf{r}, t) \right) \hat{a}_t^\dagger \right] = \hat{a}_k \]
and
\[ \int d\mathbf{r} \left( -v_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) + u_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) \right) = \sum_t \left[ \int d\mathbf{r} \left( u_k(\mathbf{r}, t) v_l(\mathbf{r}, t) - v_k(\mathbf{r}, t) u_l(\mathbf{r}, t) \right) \hat{a}_t \right. \\
+ \left. \int d\mathbf{r} \left( u_k(\mathbf{r}, t) u_l(\mathbf{r}, t) - v_k(\mathbf{r}, t) v_l(\mathbf{r}, t) \right) \hat{a}_t^\dagger \right] = \hat{a}_k^\dagger \]
by the normalisation condition (A.9) and the symmetry conditions (A.10) and (A.11).

Therefore the inverse Bogoliubov transformation is given by
\[ \hat{a}_k = \int d\mathbf{r} \left( u^*_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) - v^*_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) \right) \]
with Hermitian conjugate
\[ \hat{a}_k^\dagger = \int d\mathbf{r} \left( -v_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) + u_k(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) \right). \]

It is easy to verify that
\[ \left[ \hat{a}_k, \hat{a}_l^\dagger \right] = \int d\mathbf{r} d\mathbf{r}' \left( u^*_k(\mathbf{r}, t) u_l(\mathbf{r}', t) - v_k(\mathbf{r}, t) v^*_l(\mathbf{r}', t) \right) \delta(\mathbf{r} - \mathbf{r}') = \delta_{k,l} \]
\[ \left[ \hat{a}_k, \hat{a}_l \right] = \int d\mathbf{r} d\mathbf{r}' \left( u^*_k(\mathbf{r}, t) v_l(\mathbf{r}', t) - v^*_k(\mathbf{r}, t) u_l(\mathbf{r}', t) \right) \delta(\mathbf{r} - \mathbf{r}') = 0 \]
and
\[ \left[ \hat{a}_k^\dagger, \hat{a}_l^\dagger \right] = \int d\mathbf{r} d\mathbf{r}' \left( u_k(\mathbf{r}, t) v^*_l(\mathbf{r}', t) - v_k(\mathbf{r}, t) u^*_l(\mathbf{r}', t) \right) \delta(\mathbf{r} - \mathbf{r}') = 0 \]
thereby preserving the commutation relations (A.6) showing that the transformation is indeed canonical.

### A.1.3 Diagonalisation of the HFB Hamiltonian

The purpose of making the Bogoliubov transformation is to diagonalise the quadratic approximation \( \hat{H}_{\text{HFB}} \) of the Grand-Canonical Hamiltonian \( \hat{H}^{\text{GC}} \). This, together with the commutation relations (A.6), (A.7) and (A.8) led to the time-dependent HFB equations (2.62) and (2.63), and hence to the time-independent HFB equations (2.65) and (2.66). We now show that these equations diagonalise the HFB Hamiltonian \( \hat{H}_{\text{HFB}} \) given by equation (2.57), namely
\[ \hat{H}_{\text{HFB}}(t) = \hat{H}_{\text{HFB}_0}(t) + \hat{H}_{\text{HFB}_1}(t) + \hat{H}_{\text{HFB}_2}(t) \]
where $\dot{H}_{HFB_0}(t)$, $\dot{H}_{HFB_1}(t)$ and $\dot{H}_{HFB_2}(t)$ are given by equations (2.58), where $\dot{H}_{HFB_1}(t)$ and $\dot{H}_{HFB_2}(t)$ may also be written in the forms (4.32) and (4.33) respectively. Substituting the time-independent BdGEs (2.66) into the above equation we find that
\[
\Delta \mu \Phi(r) = \left(\hat{h}(r) - \mu + g \left(|\Phi(r)|^2 + 2\bar{n}(r)\right)\right) \Phi(r) + g\bar{m}(r)\Phi^*(r)
\]
into $\dot{H}_{HFB_1}(t)$ (4.32)
\[
\dot{H}_{HFB_1}(t) = \int dr \left(\frac{1}{2} \hat{\eta}^\dagger \left(\hat{h} - \mu + g \left(|\Phi|^2 + \bar{n}\right)\right) \hat{\eta} + g \left(\Phi^2 + \bar{m}\right) \hat{\eta}^\dagger \right) + \text{h.c.}
\]
we find in the time-independent situation that
\[
\dot{H}_{HFB_1} = \Delta \mu \int dr \left(\Phi \hat{\eta}^\dagger - \Phi^* \hat{\eta}\right).
\]
So $\dot{H}_{HFB_1} = 0$ for $\Delta \mu = 0$. By (4.33)
\[
\dot{H}_{HFB_2}(t) = \int dr \left(\frac{1}{2} \hat{\eta}^\dagger \left(\hat{h} - \mu + 2g \left(|\Phi|^2 + \bar{n}\right)\right) \hat{\eta} + g \left(\Phi^2 + \bar{m}\right) \hat{\eta}^\dagger \right) + \text{h.c.}
\]
and substituting the Boboliubov transformation (A.4), and its Hermitian conjugate (A.5) and the time-independent BdGEs (2.66) into the above equation we find that
\[
\dot{H}_{HFB_2} = \frac{1}{2} \sum_{qr} \epsilon_r \left[\hat{a}_q \hat{a}_r \int dr \left(v_q u_r - u_q v_r\right) + \hat{a}_q^\dagger \hat{a}_r \int dr \left(u_q v_r^* - v_q u_r^*\right) - \delta_{qr} \int dv_q v_r^* \right. \\
+ \left. \hat{a}_q^\dagger \hat{a}_r \int dr \left(u_q^* u_r - v_q^* v_r\right) - \delta_{qr} \int dv_q v_r^*\right] + \hat{a}_q^\dagger \hat{a}_r \int dr \left(u_q^* v_r^* - v_q^* u_r^*\right)
\]
Applying the symmetry relations (A.10) and (A.11), and the normalisation condition (A.9), we obtain
\[
\dot{H}_{HFB_2} = \sum_q \epsilon_q \left(\hat{n}_q - \int dr \left|v_q\right|^2\right),
\]
and therefore for $\Delta \mu = 0$,
\[
\dot{H}_{HFB} = \int dr \left(\Phi^* \left(\hat{h} - \mu + \frac{g}{2} |\Phi|^2\right) \Phi - g \left(\bar{n}^2(r) + \frac{1}{2} |\bar{m}(r)|^2\right)\right) + \sum_k \epsilon_k \hat{n}_k - \sum_k \epsilon_k \int dr \left|v_k\right|^2
\]
showing that the HFB equations diagonalise the HFB Hamiltonian.

### A.2 Orthogonal HFB

#### A.2.1 Commutation Relations for Bose Field Operators

In the orthogonal HFB formalism presented in chapter 4.3, we separated the Bose field operator $\hat{\psi}(r,t)$ into a coherent part represented by the condensate field operator $\hat{\Phi}(r,t)$ and an incoherent part represented by the fluctuation field operator $\hat{\eta}(r,t)$
\[
\hat{\psi}(r,t) = \hat{\Phi}(r,t) + \hat{\eta}(r,t).
\]
Appendix A. Properties of the HFB and Orthogonal HFB Formalism

We write the coherent field $\hat{\Phi}(\mathbf{r}, t)$ in terms of a condensate field annihilation operator and a condensate wave-function as

$$\hat{\Phi}(\mathbf{r}, t) \equiv \phi(\mathbf{r}, t) \hat{a}_c(t)$$  \hspace{1cm} (A.13)

with $\hat{a}_c(t)$ and $\hat{a}_c^\dagger(t)$ being respectively the annihilation and creation operators for the condensate, and $\phi(\mathbf{r}, t)$ some condensate wavefunction which satisfies the normalisation condition

$$\int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 = 1,$$  \hspace{1cm} (A.14)

and where

$$\hat{\eta}(\mathbf{r}, t) \equiv \hat{\psi}(\mathbf{r}, t) - \phi(\mathbf{r}, t) \int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t)$$  \hspace{1cm} (A.15)

is the fluctuation operator for the incoherent (thermal) part. Then as we saw in chapter 4.3,

$$\int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) = \int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) - \int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 \int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) = 0$$

by the normalisation condition (A.14), thus we satisfy the orthogonality condition

$$\int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\eta}(\mathbf{r}, t) = 0$$  \hspace{1cm} (A.16)

so the condensate and thermal populations are orthogonal, as required. Multiplying both sides of (A.15) by $\phi^*(\mathbf{r}, t)$ and integrating over all space, we find that

$$\hat{a}_c(t) = \int d\mathbf{r} \phi^*(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t).$$  \hspace{1cm} (A.17)

Let us define the projection operator

$$Q(\mathbf{r}, \mathbf{r}') \equiv \delta(\mathbf{r} - \mathbf{r}') - \phi(\mathbf{r}, t)\phi^*(\mathbf{r}', t).$$  \hspace{1cm} (A.18)

We now show that the commutation relations (4.80) - (4.85) hold:

1. To show (4.80), we note that since $\hat{\psi}(\mathbf{r}, t)$ is a Bose field operator, it satisfies the usual Bose commutation relations (A.1) and therefore by (A.17)

$$[\hat{a}_c(t), \hat{a}_c^\dagger(t)] = \int d\mathbf{r} d\mathbf{r}' \phi^*(\mathbf{r}, t) \phi(\mathbf{r}', t) \left[ \hat{\psi}(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t) \right] = \int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 = 1$$

by normalisation condition (A.14), and

$$[\hat{a}_c(t), \hat{a}_c(t)] = \int d\mathbf{r} d\mathbf{r}' \phi^*(\mathbf{r}, t) \phi(\mathbf{r}', t) \left[ \hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t) \right] = 0.$$  

Similarly

$$[\hat{a}_c^\dagger(t), \hat{a}_c^\dagger(t)] = 0,$$

and therefore (4.80) holds.
Appendix A. Properties of the HFB and Orthogonal HFB Formalism

2. By equation (A.15)
   \[ [\hat{\eta}(r, t), \hat{\eta}^\dagger(r', t)] = \int dr' \phi^*(r', t) \left[ \hat{\psi}(r', t), \hat{\psi}^\dagger(r, t) \right] \]
   \[ -\phi^*(r', t) \int dr'' \phi^*(r'', t) \left[ \hat{\psi}(r', t), \hat{\psi}^\dagger(r'', t) \right] \]
   \[ +\phi(r, t)\phi^*(r', t) \int dr''dr''' \phi^*(r'', t)\phi(r'''', t) \left[ \hat{\psi}(r'', t), \hat{\psi}^\dagger(r'''', t) \right] \]
   \[ = \delta(r - r') - \phi^*(r, t)\phi(r', t) = Q(r, r', t) \]

by (A.18). Clearly
\[ [\hat{\eta}(r, t), \hat{\eta}^\dagger(r', t)] = [\hat{\eta}^\dagger(r, t), \hat{\eta}^\dagger(r', t)] = 0 \]

from the Bose commutation relations (A.1) for the Bose field operator \( \hat{\psi}(r, t) \), thereby proving (4.81).

3. By equations (A.17) and the Bose commutation relations (A.1)
   \[ \left[ \hat{a}_c(t), \hat{\psi}(r, t) \right] = \int dr' \phi^*(r', t) \left[ \hat{\psi}(r', t), \hat{\psi}(r, t) \right] = 0, \]
   \[ \left[ \hat{a}_c^\dagger(t), \hat{\psi}^\dagger(r, t) \right] = \int dr' \phi^*(r', t) \left[ \hat{\psi}(r', t), \hat{\psi}^\dagger(r, t) \right] = \phi^*(r, t), \]
   \[ \left[ \hat{a}_c^\dagger(t), \hat{\psi}^\dagger(r, t) \right] = \int dr' \phi(r', t) \left[ \hat{\psi}^\dagger(r', t), \hat{\psi}^\dagger(r, t) \right] = 0, \]

and
\[ \left[ \hat{a}_c^\dagger(t), \hat{\psi}(r, t) \right] = \int dr' \phi(r', t) \left[ \hat{\psi}^\dagger(r', t), \hat{\psi}(r, t) \right] = -\phi(r, t). \]

So
\[ [\hat{a}_c(t), \hat{\eta}(r, t)] = \left[ \hat{a}_c(t), \hat{\psi}(r, t) \right] - [\hat{a}_c(t), \hat{a}_c(r, t)] \phi(r, t) = 0, \]
\[ [\hat{a}_c^\dagger(t), \hat{\eta}^\dagger(r, t)] = \left[ \hat{a}_c^\dagger(t), \hat{\psi}^\dagger(r, t) \right] - [\hat{a}_c^\dagger(t), \hat{a}_c^\dagger(r, t)] \phi^*(r, t) = 0, \]
\[ [\hat{a}_c(t), \hat{\eta}^\dagger(r, t)] = \left[ \hat{a}_c(t), \hat{\psi}^\dagger(r, t) \right] - [\hat{a}_c(t), \hat{a}_c^\dagger(r, t)] \phi^*(r, t) = 0, \]

and
\[ [\hat{a}_c^\dagger(t), \hat{\eta}(r, t)] = \left[ \hat{a}_c^\dagger(t), \hat{\psi}(r, t) \right] - [\hat{a}_c^\dagger(t), \hat{a}_c(t)] \phi(r, t) = 0. \]

thus proving (4.82) and (4.83).

4. Hence (4.84) follows since \( \hat{\Phi}(r, t) \equiv \phi(r, t)\hat{a}_c(t) \) by (A.13).

5. Since \( \hat{\psi}(r, t) = \hat{\Phi}(r, t) + \hat{\eta}(r, t) \) by equation (A.12), we have from the commutation relations (A.1) and (4.84)
   \[ [\hat{\eta}(r, t), \hat{\psi}(r', t)] = \left[ \hat{\psi}(r, t), \hat{\psi}(r', t) \right] - \left[ \hat{\Phi}(r, t), \hat{\psi}(r', t) \right] = 0, \]

and
\[ [\hat{\eta}(r, t), \hat{\psi}^\dagger(r', t)] = \left[ \hat{\psi}(r, t), \hat{\psi}^\dagger(r', t) \right] - \left[ \hat{\Phi}(r, t), \hat{\psi}^\dagger(r', t) \right] = \delta(r - r') - \phi(r, t)\phi^*(r', t) = Q(r, r') \]

thereby proving (4.85).
A.2.2 Symmetry and Orthogonality Properties of the Bogoliubov Transformation

We assume that the same symmetry and orthogonality properties of the Bogoliubov transformation (A.4) and (A.5), given by equations (A.10), (A.11) and (A.9) respectively, hold as for standard HFB.

A.2.3 Diagonalisation of the HFB Hamiltonian

Substituting the time-independent GGPE (4.106)

\[ \Delta \mu \Phi(r) = \left( \hat{h}(r) - \mu + g \left( |\Phi(r)|^2 + 2\hat{n}(r) \right) \right) \Phi(r) + g\hat{n}(r)\Phi^*(r) - \int dr' \hat{P}(r, r')\phi(r') \]

(A.19)

into \( \hat{H}_{HFB_1}(t) \) as given by equation (4.32) we find in the time-independent situation that

\[ \hat{H}_{HFB_1} = \Delta \mu \int dr \left( \hat{\eta}^\dagger \Phi + \Phi^* \hat{\eta} \right) + \int dr \left( \hat{\eta}^\dagger \int dr' \hat{P}(r, r')\phi(r') + \text{h.c.} \right) \approx \Delta \mu \int dr \left( \hat{\eta}^\dagger \Phi + \Phi^* \hat{\eta} \right) \]

to quadratic order in the fluctuation operator \( \hat{\eta} \), and therefore \( \hat{H}_{HFB_1} = 0 \) for \( \Delta \mu = 0 \). In view of the orthogonality condition (4.77), we can write

\[ \hat{H}_{HFB_2}(t) = \int dr \left\{ \frac{1}{2} \hat{\eta}^\dagger(r) \int dr' Q(r, r') \left[ \left( \hat{h}(r') - \mu + g \left( |\Phi(r')|^2 + 2\hat{n}(r') \right) \right) \hat{\eta}(r') \right. \right. \\
+ g \left( \Phi^2(r') + \tilde{m}(r') \right) \hat{\eta}^\dagger(r') \right. \\
+ \frac{1}{2} \int dr' Q(r, r') \left[ \left( \hat{h}^*(r') - \mu + g \left( |\Phi(r')|^2 + 2\hat{n}(r') \right) \right) \hat{\eta}^\dagger(r') \right. \\
+ g \left( \Phi^2(r') + \tilde{m}^*(r') \right) \hat{\eta}(r') \left\} \hat{\eta}(r) \right\} \]

and substituting the Boboliubov transformation (A.4), and its Hermitian conjugate (A.5) and the time-independent BdGEs (4.107) into the above equation we find that

\[ \hat{H}_{HFB_2} = \frac{1}{2} \sum_q \epsilon_r \left[ \hat{a}_q^\dagger \hat{a}_r \int dr \left( v_q u_r - u_q v_r \right) + \hat{a}_q^\dagger \hat{a}_q \int dr \left( u_q u_r^* - v_q v_r^* \right) - \delta_{qr} \int dv v_q v_r^* \right. \\
+ \hat{a}_q^\dagger \hat{a}_r \int dr \left( u_r^* u_q - v_r^* v_q \right) - \delta_{rq} \int dv v_r v_q^* + \hat{a}_q^\dagger \hat{a}_r \int dr \left. \left( u_q^* v_r - v_q^* u_r \right) \right] \]

as before. Applying the symmetry relations (A.10) and (A.11), and the orthogonality relation (A.9), we obtain

\[ \hat{H}_{HFB_2} = \sum_q \epsilon_q \left( \hat{n}_q - \int dr |v_q|^2 \right) \]

and therefore for \( \Delta \mu = 0 \),

\[ \hat{H}_{HFB} = \int dr \left( \Phi^* \left( \hat{h} - \mu + \frac{g}{2} |\Phi|^2 \right) \Phi - g \left( \hat{n}(r) + \frac{1}{2} |\tilde{m}(r)|^2 \right) \right) + \sum_k \epsilon_k \hat{n}_k - \sum_k \epsilon_k \int dr |v_k|^2 \]
Appendix A. Properties of the HFB and Orthogonal HFB Formalism

showing that the orthogonal HFB equations diagonalise the HFB Hamiltonian. Substituting the time-independent generalised GGPEs (A.19) into this equation gives us

$$\hat{H}_{HFB} = \int dr \Phi^* \left( -g \left( \frac{1}{2} |\Phi|^2 + 2\tilde{n} \right) \Phi - g\tilde{m}\Phi^* \right. $$

$$\left. - g \left( \tilde{n}(r) + \frac{1}{2} |\tilde{m}(r)|^2 \right) + \sum_k \epsilon_k \hat{n}_k - \sum_k \epsilon_k \int dr |v_k|^2, \right) $$

since $\int dr \Phi^*(\mathbf{r}) \int dr' \hat{P}_k(\mathbf{r}, \mathbf{r}') \phi_k(\mathbf{r}') = 0$, and hence we obtain (for $\Delta \mu = 0$)

$$\hat{H}_{HFB} = \sum_k \epsilon_k \hat{n}_k - g \int dr \left\{ \Phi^* \left[ \left( \frac{1}{2} |\Phi|^2 + 2\tilde{n} \right) \Phi \right] + \frac{1}{2} \left( \tilde{m}\Phi^* + \tilde{m}^*\Phi^2 \right) \right.$$

$$\left. + \tilde{n} + \frac{1}{2} |\tilde{m}|^2 \right\} - \sum_k \epsilon_k \int dr |v_k|^2. \right)$$

Let us define

$$I_{HFB} = -g \int dr \left\{ \Phi^* \left[ \left( \frac{1}{2} |\Phi|^2 + 2\tilde{n} \right) \Phi \right] + \frac{1}{2} \left( \tilde{m}\Phi^* + \tilde{m}^*\Phi^2 \right) \right.$$

$$\left. + \tilde{n} + \frac{1}{2} |\tilde{m}|^2 \right\} - \sum_k \epsilon_k \int dr |v_k|^2. \right)$$

Then this simplifies to

$$\hat{H}_{HFB} = I_{HFB} + \sum_k \epsilon_k \hat{n}_k. \right)$$

For $\Delta \mu \neq 0$ we find that

$$\hat{H}_{HFB} = I_{HFB} + \Delta \mu \int dr \left( \hat{\eta}^\dagger \Phi + \Phi^* \hat{\eta} \right) + N_c \Delta \mu + \sum_k \epsilon_k \hat{n}_k. \right)$$

A.3 Condensate and Quasi-particle Occupation Numbers

We first note that given the Grand Canonical Hamiltonian $\hat{H}^{(GC)}$, the thermal average for any operator $\hat{O}$ is given by [169]

$$\langle \hat{O} \rangle = \frac{\text{Tr} \left\{ \hat{O} \exp \left( \beta \hat{H}^{(GC)} \right) \right\}}{\mathcal{Z} (\beta)} \right)$$

where $\mathcal{Z} (\beta)$ is the partition function for the Grand Canonical Hamiltonian $\hat{H}^{(GC)}$ given by

$$\mathcal{Z} (\beta) \equiv \text{Tr} \left\{ \exp \left( \beta \hat{H}^{(GC)} \right) \right\}. \right)$$

In what follows we make use of the following two results for any real number $x$ such that $|x| < 1$:

1. $\sum_{n=1}^{\infty} x^n = \frac{1}{1-x}$, and
2. \((1 - x) \sum_{n=1}^{\infty} nx^n = \frac{x}{1-x}\).

Here \(\hat{H}^{(GC)} \approx \hat{H}_{HFB} = I_{HFB} + \Delta \mu \int dr (\hat{\eta}^\dagger \Phi + \Phi^* \hat{\eta}) + N_c \Delta \mu + \sum_q \epsilon_q \tilde{n}_q\) by equation (A.23), where the integral \(I_{HFB}\) is given by equation (A.21) above, and therefore\(^1\)

\[
\mathcal{Z}(\beta) \equiv \text{Tr} \left\{ \exp (-\beta I_{HFB}) [\exp (-\beta N_c \Delta \mu)] \left[ \prod_k \exp (-\beta \tilde{n}_k \epsilon_k) \right] \right\} \quad (A.26)
\]

which we assume can be re-written as

\[
\mathcal{Z}(\beta) \approx \exp (-\beta I_{HFB}) \left[ \sum_{N_c=0}^{\infty} N_c e^{-\beta N_c \Delta \mu} \right] \left[ \prod_k \sum_{n_k=1}^{\infty} e^{-\beta n_k \epsilon_k} \right] \quad (A.27)
\]

where \(N_c\) is the condensate occupation number, and \(n_k\) is the occupation number for the \(k\)th quasi-particle excitation. We apply the definition (A.24) for the thermal average \(\langle \hat{O} \rangle\) of an operator \(\hat{O}\), and defining the thermal averages \(\bar{N}_c \equiv \langle N_c \rangle\) and \(\bar{n}_q \equiv \langle \tilde{n}_q \rangle\) for the condensate and quasi-particle number operators \(\hat{N}_c \equiv \hat{a}^\dagger \hat{a}\) and \(\hat{n}_q \equiv \hat{a}^\dagger \hat{a}\) respectively, we find (assuming that the integral \(I_{HFB}\) contains purely thermally-averaged quantities, and can therefore be factored out when tracing over Fock space) that

\[
\bar{N}_c \approx \frac{e^{-\beta I_{HFB}}}{\mathcal{Z}(\beta)} \left[ \sum_{N_c=0}^{\infty} N_c e^{-\beta N_c \Delta \mu} \right] \left[ \prod_k \sum_{n_k=1}^{\infty} e^{-\beta n_k \epsilon_k} \right] \quad (A.28)
\]

and

\[
\bar{n}_q \approx \frac{e^{-\beta I_{HFB}}}{\mathcal{Z}(\beta)} \left[ \sum_{N_c=0}^{\infty} e^{-\beta N_c \Delta \mu} \right] \left[ \prod_k \sum_{n_k=0}^{\infty} e^{-\beta n_k \epsilon_k} \right] \left[ \sum_{n_q=0}^{\infty} n_q e^{-\beta n_q \epsilon_q} \right]. \quad (A.29)
\]

Therefore by the results 1 and 2 above, we find that the thermal averages \(\bar{N}_c\) and \(\bar{n}_q\) for the condensate and quasiparticle occupation numbers obey the Bose distribution, i.e

\[
\bar{N}_c = \frac{1}{\exp (\beta \Delta \mu) - 1}
\]

and

\[
\bar{n}_q = \frac{1}{\exp (\beta \epsilon_q) - 1}.
\]

Here we drop the bars, and regard \(N_c\) as the thermal average for the occupation number for the condensate, and \(n_q\) as the thermal average for the quasi-particle number operator.

\(^1\)In what follows we assume that we can regard the quantities in \(I_{HFB}\) as thermal averages which are therefore unaffected when tracing over Fock space in evaluating the partition function \(\mathcal{Z}(\beta)\) in equation (A.26) and the quantities \(\bar{N}_c\) and \(\bar{n}_q\), and hence we can factor out the term \(\exp (-\beta I_{HFB})\) as we have done in equations (A.27), (A.28) and (A.29). We also note that the integral \(\Delta \mu \int dr (\hat{\eta}^\dagger \Phi + \Phi^* \hat{\eta})\) is traceless since \(\langle n_1 \ldots n_q \ldots | \hat{a}_q | n_1 \ldots n_q \ldots \rangle = \langle n_1 \ldots n_q \ldots | \hat{a}_p^\dagger | n_1 \ldots n_q \ldots \rangle = 0\) and therefore does not affect the calculations for ensemble averages.
Appendix A. Properties of the HFB and Orthogonal HFB Formalism

\[ \langle \hat{n}_q \rangle \equiv \langle \hat{a}_q^\dagger \hat{a}_q \rangle. \] Thus we can write the occupation number \( N_c \) for the condensate in the time-independent case as

\[ N_c = \frac{1}{\exp(\beta \Delta \mu) - 1} \] (A.30)

and the occupation number \( N_q \) for thermal mode \( q \) as

\[ N_q = \int \text{d}r \left( n_q |u_q(r)|^2 + (n_q + 1) |v_q(r)|^2 \right) \] (A.31)

by equation (2.52), where we have shown that\(^2\)

\[ n_q = \frac{1}{\exp(\beta \epsilon_q) - 1} \] (A.32)

are the occupation numbers for quasiparticle \( q \). Since by equation (A.30) the true value for the chemical potential differs from the eigenvalue for the GGPE ground state by \( \Delta \mu \), we need to consider the fugacity term \( z = \exp\left( \frac{\Delta \mu}{kT} \right) \) in the calculation of the quasi-particle occupation numbers given by \( n_q = N_{BE}(\epsilon_q) = \frac{1}{z-1} \exp(\beta \epsilon_q) \) in chapter 4, section 4.2.3, where the energies are with respect to the eigenvalue of the condensate ground state \( \mu + \Delta \mu \), and not the true chemical potential \( \mu \). Here \( \Delta \mu \) is the difference between the eigenvalue and the true chemical potential. In cases where the quasi-particle energies are given with respect to the true chemical potential, we use the expression (A.32) for the occupation numbers, i.e. \( n_q = \frac{1}{\exp(\beta \epsilon_q) - 1} \). As pointed out in chapter 4, \( \Delta \mu \) is negligible at low temperature, for large \( N_{\text{atoms}} \), hence the fugacity term \( z = \exp\left( \frac{\Delta \mu}{kT} \right) \) is very close to unity, and can therefore be ignored.

\(^2\)Note that for \( p \neq q \), \( \langle n_1 \ldots n_p \ldots n_q \ldots | \hat{a}_p^\dagger \hat{a}_q | n_1 \ldots n_p \ldots n_q \ldots \rangle = 0 \), so \( \langle \hat{a}_p^\dagger \hat{a}_q \rangle = n_q \delta_{pq} \) with \( n_q \) given by (A.32).
Appendix B

Conservation Laws for HFB and Orthogonal HFB

B.1 Vector Calculus Results applied to Bose Field Operators

B.1.1 Standard Results from Vector Calculus

Consider any volume \( V \) bounded by a surface \( S \), and let \( \phi(\mathbf{r}) \) and \( \psi(\mathbf{r}) \) be smooth scalar fields and \( \chi(\mathbf{r}) \) a smooth vector field such that \( \phi(\mathbf{r}), \psi(\mathbf{r}), \) and \( \chi(\mathbf{r}) \) and all their derivatives vanish as \( r \to \infty \). Then the following results hold:

1. By Green’s second identity, we have

\[
\int_V d\mathbf{r} \left( \phi(\mathbf{r}) \nabla^2 \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla^2 \phi(\mathbf{r}) \right) = \oint_S d\mathbf{S} \cdot \left( \phi(\mathbf{r}) \nabla \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla \phi(\mathbf{r}) \right)
\]

and since both \( \phi(\mathbf{r}) \) and \( \psi(\mathbf{r}) \) and all their derivatives vanish as \( r \to \infty \), integrating over all space implies \( \oint_S d\mathbf{S} \cdot \left( \phi(\mathbf{r}) \nabla \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla \phi(\mathbf{r}) \right) = 0 \), thus we obtain the result

\[
\int d\mathbf{r} \phi(\mathbf{r}) \nabla^2 \psi(\mathbf{r}) = \int d\mathbf{r} \psi(\mathbf{r}) \nabla^2 \phi(\mathbf{r}) \quad (B.1)
\]

where integration over all space is implied.

2. By the divergence theorem

\[
\int_V d\mathbf{r} \nabla \cdot \chi(\mathbf{r}) = \oint_S d\mathbf{S} \cdot \chi(\mathbf{r}). \quad (B.2)
\]
3. It can be shown that the following standard identity
\[ \int_V d\mathbf{r} \nabla \times \chi(\mathbf{r}) = \oint_S d\mathbf{S} \times \chi(\mathbf{r}) \] (B.3)
holds.

4. Since \( \chi(\mathbf{r}) \) and all its derivatives vanish as \( r \to \infty \), integrating over all space implies \( \oint_S d\mathbf{S} \cdot \chi(\mathbf{r}) = 0 \) and therefore by (B.2)
\[ \int d\mathbf{r} \nabla \cdot \chi(\mathbf{r}) = 0. \] (B.4)

Then for smooth scalar functions \( \phi(\mathbf{r}) \) and \( \psi(\mathbf{r}) \) and any vector \( \mathbf{v} \),
\[ \mathbf{v} \cdot \int d\mathbf{r} (\phi(\mathbf{r}) \nabla \psi(\mathbf{r}) + \psi(\mathbf{r}) \nabla \psi(\mathbf{r})) = \int d\mathbf{r} \nabla \cdot (\mathbf{v} \phi(\mathbf{r}) \psi(\mathbf{r})) = 0 \]
by (B.4) above, and therefore
\[ \mathbf{v} \cdot \int d\mathbf{r} \phi(\mathbf{r}) \nabla \phi(\mathbf{r}) = -\mathbf{v} \cdot \int d\mathbf{r} \psi(\mathbf{r}) \nabla \psi(\mathbf{r}). \] (B.5)

5. We have
\[ \nabla \times (r \phi(\mathbf{r})) = \phi(\mathbf{r}) (\nabla \times r) = \nabla \phi(\mathbf{r}) \times \mathbf{r} = -\mathbf{r} \times (\nabla \phi(\mathbf{r})) \]
since \( \nabla \times \mathbf{r} = 0 \). Then by equation (B.3), it follows that
\[ \int_V d\mathbf{r} (r \nabla) (\phi(\mathbf{r}) \psi(\mathbf{r})) = -\oint_S d\mathbf{S} \times (r \phi(\mathbf{r}) \psi(\mathbf{r})) \]
Since both \( \phi(\mathbf{r}) \) and \( \psi(\mathbf{r}) \) and all their derivatives vanish as \( r \to \infty \), integrating over all space implies \( \oint_S d\mathbf{S} \times (r \phi(\mathbf{r}) \psi(\mathbf{r})) = 0 \), and therefore for integration over all space
\[ \int d\mathbf{r} (r \nabla) (\phi(\mathbf{r}) \psi(\mathbf{r})) = 0 \]
and therefore
\[ \int d\mathbf{r} \phi(\mathbf{r}) (r \nabla) \psi(\mathbf{r}) = -\int d\mathbf{r} \psi(\mathbf{r}) (r \nabla) \phi(\mathbf{r}). \] (B.6)

## B.1.2 Vector Calculus Results for Bose Field Operators

Let \( \hat{\psi}(\mathbf{r}, t) \) be a Bose field operator written as the sum of a condensate operator \( \hat{\Phi}(\mathbf{r}, t) \) corresponding to the coherent part, and a fluctuation operator part corresponding to the thermal cloud (incoherent part), i.e. as \( \hat{\psi}(\mathbf{r}, t) = \hat{\Phi}(\mathbf{r}, t) + \hat{\eta}(\mathbf{r}, t) \). We consider here standard and orthogonal HFB where we assume a macroscopic occupation of the condensate, thus
Appendix B. Conservation Laws for HFB and Orthogonal HFB

Φ(r, t) = ⟨Φ(r, t)⟩ is the condensate wave-function. The fluctuation operator \( \hat{\eta}(r, t) \) can be written in the quasi-particle basis using the Bogoliubov transformation (2.43)

\[
\hat{\eta}(r, t) = \sum_k \left( u_k(r, t) \hat{a}_k + v^*_k(r, t) \hat{a}^+_k \right)
\]

where the \( \hat{a}^+_k \) and the \( \hat{a}_k \) are respectively the quasi-particle creation and annihilation operators with the corresponding quasi-particle amplitude wave-functions \( u_k(r, t) \) and \( v^*_k(r, t) \).

Let \( \hat{h}_\Omega(r) \) be the single-particle Hamiltonian in the rotating frame, and \( \hat{h}_\nu(r) \) be the single-particle Hamiltonian in the rotating frame as defined in chapters 2 and 4. Then the following results hold:

1. For the Bose field operator \( \hat{\psi}(r, t) \)

\[
\left\langle \int \! dr \left( \hat{\psi}^\dagger(r, t) \hat{h}_\Omega(r) \hat{\psi}(r, t) - \left( \hat{h}^*_\Omega(r) \hat{\psi}^\dagger(r, t) \right) \hat{\psi}(r, t) \right) \right\rangle = 0 \tag{B.8}
\]

2. For any linear differential operator \( \hat{D}(r) \)

\[
\left\langle \int \! dr \left( \hat{\psi}^\dagger \hat{D} \left( \hat{h}_\Omega \hat{\psi} \right) - \left( \hat{h}^*_\Omega \hat{\psi}^\dagger \right) \hat{D} \hat{\psi} \right) \right\rangle = \int \! dr \left( |\Phi|^2 + \bar{n} \right) \hat{D}V_T \tag{B.9}
\]

where \( V_T(r) \) is the trapping potential of the BEC.

3. For the Bose field operator \( \hat{\psi}(r, t) \)

\[
\left\langle \int \! dr \left( \hat{\psi}^\dagger(r, t) \hat{h}_\nu(r) \hat{\psi}(r, t) - \left( \hat{h}^*_\nu(r) \hat{\psi}^\dagger(r, t) \right) \hat{\psi}(r, t) \right) \right\rangle = 0 \tag{B.10}
\]

4. For any linear differential operator \( \hat{D}(r) \)

\[
\left\langle \int \! dr \left( \hat{\psi}^\dagger \hat{D} \left( \hat{h}_\nu \hat{\psi} \right) - \left( \hat{h}^*_\nu \hat{\psi}^\dagger \right) \hat{D} \hat{\psi} \right) \right\rangle = \int \! dr \left( |\Phi|^2 + \bar{n} \right) \hat{D}V_T \tag{B.11}
\]

where \( V_T(r) \) is the trapping potential of the BEC.

We now show that these results are true:

1. Proof of result 1:

\[
\left\langle \int \! dr \left( \hat{\psi}^\dagger \hat{h}_\Omega \hat{\psi} - \left( \hat{h}^*_\Omega \hat{\psi}^\dagger \right) \hat{\psi} \right) \right\rangle = \int \! dr \left( \Phi^* \hat{h}_\Omega \Phi - \Phi \hat{h}^*_\Omega \Phi^* \right) + \left\langle \int \! dr \left( \hat{\eta}^\dagger \hat{h}_\Omega \hat{\eta} - \left( \hat{h}^*_\Omega \hat{\eta}^\dagger \right) \hat{\eta} \right) \right\rangle
\]
We first show that for any complex scalar fields \( \phi(r, t) \) and \( \psi(r, t) \)

\[
\int d\mathbf{r} \left( \phi(r, t) \dot{h}_\Omega(r) \psi(r, t) - \psi(r, t) \dot{h}_\Omega^+(r) \phi(r, t) \right) = 0 \tag{B.12}
\]

First note that the result \( \int d\mathbf{r} \left( \phi \nabla^2 \psi - \psi \nabla^2 \phi \right) = 0 \) follows by applying equation (B.1) to the real and imaginary parts of \( \phi(r, t) \) and \( \psi(r, t) \). We also note that

\[
\int d\mathbf{r} \left( \phi (\mathbf{r} \times \nabla) \psi + \psi (\mathbf{r} \times \nabla) \phi \right) = \int d\mathbf{r} \left( (\mathbf{r} \times \nabla) (\phi \psi) \right) = 0
\]

follows by applying equation (B.6) to the real and imaginary parts of \( \phi(r, t) \psi(r, t) \) and clearly \( \int d\mathbf{r} \left( \phi V_T \psi - \psi V_T \phi \right) = 0 \). Therefore the result \( \int d\mathbf{r} \left( \phi \ddot{h}_\Omega \psi - \psi \ddot{h}_\Omega^+ \phi \right) = 0 \) holds for any complex scalar fields \( \phi(r) \) and \( \psi(r) \) where the single-particle Hamiltonian in the rotating frame for trapping potential \( V_T(r) \) is given by

\[
\dot{h}_\Omega(r) = -\frac{\hbar^2}{2m} \nabla^2 + i\hbar \mathbf{\Omega} \cdot (\mathbf{r} \times \nabla) + V_T(r). \tag{B.13}
\]

The result

\[
\int d\mathbf{r} \left( \Phi^* \dot{h}_\Omega \Phi - \Phi \dot{h}_\Omega^+ \Phi^* \right) = 0 \tag{B.14}
\]

then follows. We now show that

\[
\int d\mathbf{r} \left( \hat{\eta}^\dagger \dot{h}_\Omega \hat{\eta} - \left( \dot{h}_\Omega^+ \hat{\eta}^\dagger \right) \hat{\eta} \right) = 0 \tag{B.15}
\]

thereby verifying equation (B.8). Using equation (B.7) and its Hermitian conjugate, we see that

\[
\int d\mathbf{r} \left( \hat{\eta}^\dagger \dot{h}_\Omega \hat{\eta} - \left( \dot{h}_\Omega^+ \hat{\eta}^\dagger \right) \hat{\eta} \right) = \sum_{kl} \left[ \int d\mathbf{r} \left( v_k \dot{h}_\Omega u_l - u_l \dot{h}_\Omega^+ v_k \right) \hat{a}_k \hat{a}_l^\dagger \\
+ \int d\mathbf{r} \left( v_k \dot{h}_\Omega^+ v_l^\dagger - v_l^\dagger \dot{h}_\Omega^+ v_k \right) \hat{a}_l \hat{a}_k^\dagger \\
+ \int d\mathbf{r} \left( u_l \dot{h}_\Omega^+ u_k^\dagger - u_k^\dagger \dot{h}_\Omega^+ u_l \right) \hat{a}_k \hat{a}_l^\dagger \\
+ \int d\mathbf{r} \left( u_l^\dagger \dot{h}_\Omega^+ v_k^\dagger - v_k^\dagger \dot{h}_\Omega^+ u_l^\dagger \right) \hat{a}_k^\dagger \hat{a}_l^\dagger \right] = 0
\]

by equation (B.12), thus proving result 1 (equation (B.8)).

2. Proof of result 2:

\[
\begin{aligned}
&\left\langle \int d\mathbf{r} \left( \hat{\psi}^\dagger \hat{D} \left( \dot{h}_\Omega \hat{\psi} \right) - \left( \dot{h}_\Omega^+ \hat{\psi}^\dagger \right) \left( \hat{D} \hat{\psi} \right) \right) \right\rangle = \int d\mathbf{r} \left( \Phi^* \hat{D} \left( \dot{h}_\Omega \Phi \right) - \left( \dot{h}_\Omega^+ \Phi^* \right) \left( \hat{D} \Phi \right) \right) \\
&+ \left\langle \int d\mathbf{r} \left( \hat{\eta}^\dagger \hat{D} \left( \dot{h}_\Omega \hat{\eta} \right) - \left( \dot{h}_\Omega^+ \hat{\eta}^\dagger \right) \left( \hat{D} \hat{\eta} \right) \right) \right\rangle
\end{aligned} \tag{B.17}
\]

We first show that for any complex scalar fields \( \phi(r) \) and \( \psi(r) \)

\[
\int d\mathbf{r} \left( \phi \dot{D} \left( \dot{h}_\Omega \psi \right) - \left( \dot{h}_\Omega^+ \phi \right) \left( \hat{D} \psi \right) \right) = \int d\mathbf{r} \psi \phi \dot{D} V_T. \tag{B.18}
\]
Note that
\[
\int dr \left( (\nabla^2 \phi) (\hat{D} \psi) - \phi \hat{D} (\nabla^2 \psi) \right) = \int dr \left( (\nabla^2 \phi) (\hat{D} \psi) - \phi \nabla^2 (\hat{D} \psi) \right) = 0
\]
by applying equation (B.1) to the real and imaginary parts of \(\phi(\mathbf{r})\) and \(\psi(\mathbf{r})\). Furthermore
\[
\int dr \left( (\mathbf{r} \times \nabla) \phi \right) (\hat{D} \psi) + \phi \hat{D} ((\mathbf{r} \times \nabla) \psi) = \int dr (\mathbf{r} \times \nabla) \left( \phi \hat{D} \psi \right) = 0
\]
by applying equation (B.6) to the real and imaginary parts of \(\phi(\mathbf{r}, t)\psi(\mathbf{r}, t)\). Now
\[
\int dr \left( \phi \hat{D} (V_T \psi) - (V_T \phi) \hat{D} \psi \right) = \int dr \phi \psi \hat{D} V_T
\]
thereby proving equation (B.18). We can apply this directly to the first part of equation (B.17) showing that
\[
\int dr \left( \Phi^* \hat{D} (\hat{h}_\Omega \Phi) - (\hat{h}_\Omega^* \Phi^*) (\hat{D} \Phi) \right) = \int dr |\Phi|^2 \hat{D} V_T.
\]
Now
\[
\left\langle \int dr \left( \hat{n}^i \hat{D} \left( \hat{h}_\Omega \hat{n} \right) - \left( \hat{h}_\Omega^* \hat{n}^i \right) (\hat{D} \hat{n}) \right) \right\rangle = \sum_{kl} \int dr \left( \hat{n}^i \hat{h}_\Omega (\hat{D} \hat{n}_l) - \hat{n}_l \hat{h}_\Omega^* (\hat{D} \hat{n}_k) \right) \langle \hat{a}_k \hat{a}_l \rangle
\]
by equation (B.18) and noting that \(\langle \hat{a}_k \hat{a}_l \rangle = \langle \hat{a}_k^\dagger \hat{a}_l^\dagger \rangle = 0\) and \(\langle \hat{a}_k^\dagger \hat{a}_l \rangle = n_k \delta_{nk}\), and
\(\langle \hat{a}_k^\dagger \hat{a}_l^\dagger \rangle = (n_k + 1) \delta_{nk}\), showing that
\[
\left\langle \int dr \left( \hat{n}^i \hat{D} \left( \hat{h}_\Omega \hat{n} \right) - \left( \hat{h}_\Omega^* \hat{n}^i \right) (\hat{D} \hat{n}) \right) \right\rangle = \int dr \hat{n} \hat{D} V_T.
\]
Hence result 2 given by equation (B.9) follows.

3. Proof of result 3: We note from (B.5), i.e. \(\mathbf{v} \cdot \int dr \phi(\mathbf{r}) \nabla \psi(\mathbf{r}) = -\mathbf{v} \cdot \int dr \psi(\mathbf{r}) \nabla \phi(\mathbf{r})\) that
\[
\int dr \left( \phi(\mathbf{r}, t) \hat{h}_\nu(\mathbf{r}) \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \hat{h}_\nu^*(\mathbf{r}) \phi(\mathbf{r}, t) \right) = 0
\]
and hence that
\[
\left\langle \int dr \left( \hat{\psi}^i(\mathbf{r}, t) \hat{h}_\nu(\mathbf{r}) \hat{\psi}(\mathbf{r}, t) - \hat{\psi}(\mathbf{r}, t) \hat{h}_\nu^*(\mathbf{r}) \hat{\psi}^i(\mathbf{r}, t) \right) \right\rangle = 0.
\]
Appendix B. Conservation Laws for HFB and Orthogonal HFB

4. Proof of result 4: We note from (B.5), i.e. \( v \cdot \int d\mathbf{r} \phi(\mathbf{r}) \nabla \psi(\mathbf{r}) = -v \cdot \int d\mathbf{r} \psi(\mathbf{r}) \nabla \psi(\mathbf{r}) \) that
\[
\int d\mathbf{r} \left( (v \cdot \nabla \phi) \left( \hat{D} \psi \right) + \phi \hat{D} (v \cdot \nabla \psi) \right) = \int d\mathbf{r} \left( (v \cdot \nabla \phi) \left( \hat{D} \psi \right) + \phi v \cdot \nabla \left( \hat{D} \psi \right) \right) = 0
\]
and hence that
\[
\int d\mathbf{r} \left( -\left( \hat{h}^*_v \hat{\psi}^t \right) \left( \hat{D} \psi \right) + \hat{\psi}^t \hat{D} \left( \hat{h}_v \hat{\psi} \right) \right) = \int d\mathbf{r} \left( |\Phi|^2 + \tilde{n} \right) \hat{D} V_T
\]
by an argument similar to that used in the proof of result 2, thus proving result 4.

B.2 Conservation Laws for Standard HFB

B.2.1 Particle Number Conservation

In the Rotating Frame

From the GGPE (4.3) in the rotating frame, we find for the total number of condensate particles \( N_c(t) = \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^2 \) that
\[
i \hbar \frac{d}{dt} N_c = \frac{\hbar^2}{2m} \int d\mathbf{r} \left( -\Phi(\mathbf{r}, t) \hat{h}^*_v(\mathbf{r}) \Phi^*(\mathbf{r}, t) + \Phi^*(\mathbf{r}, t) \hat{h}_v(\mathbf{r}) \Phi(\mathbf{r}, t) \right)
+ g \int d\mathbf{r} \left( n_c(\mathbf{r}, t) + 2\tilde{n}(\mathbf{r}, t) \right) \left( |\Phi(\mathbf{r}, t)|^2 - |\Phi(\mathbf{r}, t)|^2 \right)
+ g \int d\mathbf{r} \left( \tilde{m}(\mathbf{r}) \Phi^2(\mathbf{r}) - \tilde{m}^*(\mathbf{r}) \Phi^2(\mathbf{r}) \right)
\]
Now \( \int d\mathbf{r} \left( -\Phi(\mathbf{r}, t) \hat{h}^*_v(\mathbf{r}) \Phi^*(\mathbf{r}, t) + \Phi^*(\mathbf{r}, t) \hat{h}_v(\mathbf{r}) \Phi(\mathbf{r}, t) \right) = 0 \) by (B.12). Therefore the rate of change in the condensate population is given by
\[
\frac{dN_c(t)}{dt} = ig \int d\mathbf{r} \left( \tilde{m}(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) - \tilde{m}^*(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) \right)
\] (B.22)
From the time-dependent BdGEs (4.4) and their complex conjugates, we find that
\[
i \hbar \frac{d}{dt} \int d\mathbf{r} |u_q(\mathbf{r}, t)|^2 = \frac{\hbar^2}{2m} \int d\mathbf{r} \left( -u_q(\mathbf{r}, t) \hat{h}^*_v(\mathbf{r}) u_q^*(\mathbf{r}, t) + u_q^*(\mathbf{r}, t) \hat{h}_v(\mathbf{r}) u_q(\mathbf{r}, t) \right)
+ 2g \int d\mathbf{r} \left( n_c(\mathbf{r}, t) + \tilde{n}(\mathbf{r}, t) \right) \left( |u_q(\mathbf{r}, t)|^2 - |u_q(\mathbf{r}, t)|^2 \right)
+ g \int d\mathbf{r} \left( \left( \Phi^2(\mathbf{r}, t) + \tilde{m}(\mathbf{r}, t) \right) v_q(\mathbf{r}, t) u_q^*(\mathbf{r}, t) \right)
- \left( \Phi^*(\mathbf{r}, t) + \tilde{m}^*(\mathbf{r}, t) \right) u_q(\mathbf{r}, t) v_q^*(\mathbf{r}, t) \right)
\]
and since \( \int d\mathbf{r} \left( -u_q \hat{h}^*_v u_q^* + u_q^* \hat{h}_v u_q \right) = 0 \) by (B.12), we obtain
\[
i \hbar \frac{d}{dt} \int d\mathbf{r} |u_q|^2 = g \int d\mathbf{r} \left( \left( \Phi^2 + \tilde{m} \right) v_q u_q^* - \left( \Phi^* \tilde{m}^* + \tilde{m}^* \right) u_q v_q^* \right).
\]
Similarly
\[ i\hbar \frac{d}{dt} \int d\mathbf{r} |v_q|^2 = g \int d\mathbf{r} \left( (\Phi^2 + \tilde{m}) v_q^* u_q - (\Phi^{*2} + \tilde{m}^*) u_q v_q^* \right) \]
Hence
\[ i\hbar \frac{d}{dt} \int d\mathbf{r} \tilde{n} = g \int d\mathbf{r} \sum_q (2n_q + 1) \int d\mathbf{r} \left( (\Phi^2 + \tilde{m}) u_q^* v_q - (\Phi^{*2} + \tilde{m}^*) u_q v_q^* \right), \]
so the rate of change in the thermal (non-condensate) population \( \tilde{N}(t) = \int d\mathbf{r} \tilde{n} \) is given by
\[ \frac{d\tilde{N}(t)}{dt} = i \frac{g}{\hbar} \int d\mathbf{r} \left( \tilde{m}^* (r, t) \Phi^2(r, t) - \tilde{m} (r, t) \Phi^{*2}(r, t) \right) = -\frac{dN_c(t)}{dt} \tag{B.23} \]
showing that particles are conserved for time-dependent HFB in the rotating frame.

In the Translating Frame

For the translating frame, we find that
\[ i\hbar \frac{d}{dt} N_c = \int d\mathbf{r} \left( -\Phi(r, t) \hat{h}_v(r) \Phi^*(r, t) + \Phi^*(r, t) \hat{h}_v^*(r) \Phi(r, t) \right) + g \int d\mathbf{r} \left( \tilde{m}(r) \Phi^{*2}(r) - \tilde{m}^*(r) \Phi^2(r) \right) \]
for the rate of change in the condensate population. Now
\[ i\hbar \frac{d}{dt} \int d\mathbf{r} |u_q|^2 = \int d\mathbf{r} \left( -u_q(r, t) \hat{h}_v(r) u_q^*(r, t) + u_q^*(r, t) \hat{h}_v^*(r) u_q(r, t) \right) + g \int d\mathbf{r} \left( (\Phi^2 + \tilde{m}) v_q^* u_q - (\Phi^{*2} + \tilde{m}^*) u_q v_q^* \right) \]
since \( \int d\mathbf{r} \left( -\Phi \hat{h}_v \Phi^* + \Phi^* \hat{h}_v^* \Phi \right) = 0 \) and \( \int d\mathbf{r} \left( -u_q \hat{h}_v u_q^* + u_q^* \hat{h}_v^* u_q \right) = 0 \) by (B.21) above. Similarly
\[ i\hbar \frac{d}{dt} \int d\mathbf{r} |v_q|^2 = g \int d\mathbf{r} \left( (\Phi^2 + \tilde{m}) v_q^* u_q - (\Phi^{*2} + \tilde{m}^*) u_q v_q^* \right) \]
and therefore we find as before, that the rate of change in the thermal population is given by
\[ \frac{d\tilde{N}(t)}{dt} = i \frac{g}{\hbar} \int d\mathbf{r} \left( \tilde{m}^* (r, t) \Phi^2(r, t) - \tilde{m} (r, t) \Phi^{*2}(r, t) \right) = -\frac{dN_c(t)}{dt} \]
showing that particles are also conserved in the translating frame for time-dependent HFB.

It is evident from the above discussion that particles are conserved in general for HFB.
Appendix B. Conservation Laws for HFB and Orthogonal HFB

Presence of an out-coupling potential $iV_c(r)$ as in chapter 6.

Introducing an imaginary out-coupling potential $iV_c(r)$ allows particles to be coupled into/out of the BEC. From equations (6.1), (6.2) and (6.3), we see that the out-coupling potential $iV_c(r)$ contributes an amount

$$\frac{1}{i} \int dr (\Phi^*(r,t)iV_c(r)\Phi(r,t) + iV_c(r)\Phi^*(r,t)\Phi(r,t)) = 2 \int dr V_c(r)n_c(r,t)$$

to the rate of change of condensate particles, and an amount

$$\frac{1}{i} \sum_q \left[ n_q \int dr (u_q^*iV_c u_q + iV_c u_q^* u_q) + (n_q + 1) \int dr (v_q^*iV_c v_q + iV_c v_q^* v_q) \right] = 2 \int dr \tilde{n}$$

to the rate of change of thermal particles. Hence the rate of change of condensate particles is given by

$$\frac{dN_c}{dt} = \frac{2}{\hbar} \int V_c(r)n_c(r)dr + \frac{ig}{\hbar} \int \left( \tilde{n}(r)\Phi^2(r) - \tilde{m}^*(r)\Phi^2(r) \right) dr \quad (B.24)$$

and the rate of change of the thermal population by

$$\frac{d\tilde{N}}{dt} = \frac{2}{\hbar} \int V_c(r)\tilde{n}(r)dr - \frac{ig}{\hbar} \int \left( \tilde{m}(r)\Phi^2(r) - \tilde{m}^*(r)\Phi^2(r) \right) dr \quad (B.25)$$

where $N_c$ is the total number of condensate particles and $\tilde{N}$ the total number of thermal particles. Then if we define $N_{tot}$ to be the total number of particles in the BEC, we find that the rate at which particles are coupled out of the BEC is given by

$$\frac{dN_{tot}}{dt} = \frac{2}{\hbar} \int V_c(r)n_{tot}(r)dr. \quad (B.26)$$

We note that in the absence of the out-coupling potential

$$\frac{dN_{tot}}{dt} = 0 \quad (B.27)$$

hence the total number of particles is conserved.

Violation of Particle Conservation for Popov, and for G1 and G2 Gapless Theories

We show that particle conservation is violated for the Popov approximation, and for the gapless G1 and G2 theories. The time-dependent GGPE and BdGEs may be written for Popov, G1 and G2 as (c.f. equations (2.74)-(2.80))

$$i\hbar \frac{\partial \Phi(r,t)}{\partial t} = \left( \hat{h}(r) + U_c(r,t) |\Phi(r,t)|^2 + 2U_e(r,t)\tilde{n}(r,t) \right) \Phi(r,t) \quad (B.28)$$
Appendix B. Conservation Laws for HFB and Orthogonal HFB

and

\[ i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \begin{bmatrix} \hat{L}_G(r, t) & \mathcal{M}_G(r, t) \\ -\mathcal{M}_G^*(r, t) & -\hat{L}_G^*(r, t) \end{bmatrix} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} \]  

where

\[ \hat{L}_G(r, t) \equiv \hat{h}(r) - \mu + 2U_e(r, t)|\Phi(r, t)|^2 + 2U_e(r, t)\tilde{n}(r, t) \]

\[ \mathcal{M}_G(r, t) \equiv U_e(r, t)\Phi^2(r, t) \]

with

\[ U_e(r, t) = g \left(1 + a\frac{\tilde{m}(r, t)}{\Phi^2(r, t)}\right) \]  

and

\[ U_e(r, t) = g \left(1 + b\frac{\tilde{m}(r, t)}{\Phi^2(r, t)}\right) \]

where

\[ a = \begin{cases} 0 & \text{Popov} \\ 1 & \text{G1} \\ 1 & \text{G2} \end{cases} \]  

and

\[ b = \begin{cases} 0 & \text{Popov} \\ 0 & \text{G1} \\ 1 & \text{G2} \end{cases} \]

This can be re-written in the form

\[ i\hbar \frac{\partial \Phi(r, t)}{\partial t} = \left(\hat{h}(r) - \mu + g \left(|\Phi(r, t)|^2 + 2\tilde{n}(r, t)\right)\right)\Phi(r, t) + ga\tilde{m}(r, t)\Phi^*(r, t) + 2bg\frac{\tilde{m}(r, t)\tilde{n}(r, t)}{\Phi(r, t)} \]  

and

\[ i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} = \begin{bmatrix} \hat{L}_G(r, t) & \mathcal{M}_G(r, t) \\ -\mathcal{M}_G^*(r, t) & -\hat{L}_G^*(r, t) \end{bmatrix} \begin{bmatrix} u_q(r, t) \\ v_q(r, t) \end{bmatrix} \]  

where

\[ \hat{L}_G(r, t) \equiv \hat{h}(r) - \mu + 2g \left(|\Phi(r, t)|^2 + \tilde{n}(r, t)\right) + 2g\tilde{m}(r, t) \left(a|\Phi(r, t)|^2 + b\tilde{n}(r, t)\right) / \Phi^2(r, t) \]

\[ \mathcal{M}_G(r, t) \equiv g \left(\Phi^2(r, t) + a\tilde{m}(r, t)\right) \]

Hence we find in the corresponding time-dependent case that

\[ \frac{dN_e}{dt} = i\frac{g}{\hbar} \int d\mathbf{r} \left(\tilde{m}\Phi^2 - \tilde{m}^*\Phi^2\right) + 2i\frac{g}{\hbar} b \int d\mathbf{r}\tilde{n} \left(\tilde{m}^*\frac{\Phi}{\Phi^*} - \tilde{m}\frac{\Phi^*}{\Phi}\right) \]  

and that

\[ \frac{d\tilde{N}}{dt} = i\frac{g}{\hbar} \int d\mathbf{r} \left(\tilde{m}^*\Phi^2 - \tilde{m}\Phi^2\right) + 2ia\frac{g}{\hbar} \int d\mathbf{r}\tilde{n} \left(\tilde{m}^*\frac{\Phi}{\Phi^*} - \tilde{m}\frac{\Phi^*}{\Phi}\right) + 2ib\frac{g}{\hbar} \int d\mathbf{r}\tilde{n}^2 \left(\tilde{m}^*\frac{\Phi}{\Phi^2} - \tilde{m}\frac{\Phi^*}{\Phi^2}\right) \].
Hence we find for Popov \((a = b = 0)\)

\[
\frac{dN_c}{dt} = 0, \quad (B.40)
\]

\[
\frac{d\tilde{N}}{dt} = i\frac{g}{\hbar} \int dr \left( \tilde{m}^* \Phi^2 - \tilde{m} \Phi^* \right), \quad (B.41)
\]

so

\[
\frac{d(N_c + \tilde{N})}{dt} = i\frac{g}{\hbar} \int dr \left( \tilde{m}^* \Phi^2 - \tilde{m} \Phi^* \right). \quad (B.42)
\]

For G1 \((a = 1, b = 0)\)

\[
\frac{dN_c}{dt} = i\frac{g}{\hbar} \int dr \left( \tilde{m}^* \Phi^* - \tilde{m} \Phi \right), \quad (B.43)
\]

\[
\frac{d\tilde{N}}{dt} = 2i\frac{g}{\hbar} \int dr \tilde{n} \left( \tilde{m}^* \frac{\Phi^*}{\Phi} - \tilde{m} \frac{\Phi}{\Phi^*} \right) + i\frac{g}{\hbar} \int dr \left( \tilde{m}^* \Phi^2 - \tilde{m} \Phi^* \right), \quad (B.44)
\]

so

\[
\frac{d(N_c + \tilde{N})}{dt} = 2i\frac{g}{\hbar} \int dr \tilde{n} \left( \tilde{m}^* \frac{\Phi^*}{\Phi} - \tilde{m} \frac{\Phi}{\Phi^*} \right). \quad (B.45)
\]

For G2 \((a = 1, b = 1)\)

\[
\frac{dN_c}{dt} = 2i\frac{g}{\hbar} \int dr \tilde{n} \left( \tilde{m}^* \frac{\Phi^*}{\Phi} - \tilde{m} \frac{\Phi}{\Phi^*} \right) + i\frac{g}{\hbar} \int dr \left( \tilde{m}^* \Phi^2 - \tilde{m} \Phi^* \right), \quad (B.46)
\]

\[
\frac{d\tilde{N}}{dt} = 2i\frac{g}{\hbar} \int dr \tilde{n} \left( \tilde{m}^* \frac{\Phi^*}{\Phi^2} - \tilde{m} \frac{\Phi}{\Phi^2} \right) + 2i\frac{g}{\hbar} \int dr \tilde{n} \left( \tilde{m}^* \frac{\Phi^*}{\Phi^2} - \tilde{m} \frac{\Phi}{\Phi^2} \right) + i\frac{g}{\hbar} \int dr \left( \tilde{m}^* \Phi^2 - \tilde{m} \Phi^* \right), \quad (B.47)
\]

so

\[
\frac{d(N_c + \tilde{N})}{dt} = 2i\frac{g}{\hbar} \int dr \tilde{n}^2 \left( \tilde{m}^* \frac{\Phi^*}{\Phi^2} - \tilde{m} \frac{\Phi}{\Phi^2} \right). \quad (B.48)
\]

Therefore particle conservation is violated in all three cases. As a consequence of this, Popov, and the G1 and G2 gapless theories are unsuitable candidates for time-dependent simulations.

\section*{B.2.2 Conservation of Energy}

\subsection*{Proof of Energy Conservation using Commutation Relations}

We show that the HFB energy is a constant of the motion in the absence of an external time-dependent potential. Consider first a BEC in the presence of a time-varying potential \(V(\mathbf{r}, t)\), i.e. \(\hat{H}_{HFB} \rightarrow \hat{H}_{HFB} + V(\mathbf{r}, t)\). Then by the Heisenberg equation of motion

\[
\frac{i\hbar}{\partial t} \hat{H}_{HFB} = [\hat{H}_{HFB}, \hat{H}_{HFB}] + \int d\mathbf{r} \left( i\hbar \frac{\partial V(\mathbf{r}, t)}{\partial t} \right) \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t),
\]

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and since any operator commutes with itself, and hence $[\hat{H}_{HFB}, \hat{H}_{HFB}] = 0$, we conclude that
\[ \frac{dE}{dt} = \left\langle \frac{d\hat{H}_{HFB}}{dt} \right\rangle = \left\langle \frac{\partial V}{\partial t} \right\rangle. \] (B.49)

In the situation where the external (trapping) potential is time-independent, (i.e. $\frac{\partial V}{\partial t}(r,t) = 0$), $\frac{dE}{dt} = \left\langle \frac{d\hat{H}_{HFB}}{dt} \right\rangle = 0$, showing that energy is conserved. We show that energy is also conserved for any perturbation scheme for HFB as follows. The full Grand-Canonical Hamiltonian may be written
\[ \hat{H}^{(GC)}(t) \equiv \hat{H}_{HFB}(t) + \Delta \hat{H}_{13}(t) + \Delta \hat{H}_{24}(t) \] (B.50)
where $\hat{H}_{HFB}(t)$ is the HFB Hamiltonian given by (2.57)
\[ \hat{H}_{HFB}(t) \equiv \tilde{\hat{H}}_{HFB_0}(t) + \tilde{\hat{H}}_{HFB_1}(t) + \tilde{\hat{H}}_{HFB_2}(t) \]
where we have broken the HFB Hamiltonian into Hamiltonians of zeroth, first and second order in terms of the annihilation and creation fluctuation operators $\hat{\eta}$ and $\hat{\eta}^\dagger$ as in equations with $\tilde{\hat{H}}_{HFB_0}(t)$ given by the first of equations (2.58), and $\tilde{\hat{H}}_{HFB_1}(t)$ and $\tilde{\hat{H}}_{HFB_2}(t)$ respectively by equations (4.32) and (4.33)

\[
\begin{align*}
\tilde{\hat{H}}_{HFB_0}(t) &\equiv \int dr \left( \Phi^* \left( \hat{\hbar} - \mu + \frac{g}{2} |\Phi|^2 \right) \Phi - g \left( \tilde{n}^2 + \frac{1}{2} |\tilde{m}|^2 \right) \right) \\
\tilde{\hat{H}}_{HFB_1}(t) &\equiv \int dr \left( \hat{\eta}^\dagger \left( \hat{\hbar} - \mu + g \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi + g\tilde{m}\Phi^* \right) + \text{h.c.} \\
\tilde{\hat{H}}_{HFB_2}(t) &\equiv \int dr \left( \frac{1}{\sqrt{2}} \hat{\eta}^\dagger \left( \hat{\hbar} - \mu + g \left( |\Phi|^2 + 2\tilde{n} \right) \right) \hat{\eta} + g \left( \Phi^2 + \tilde{m} \right) \hat{\eta} \right) + \text{h.c.} \\
\end{align*}
\]

The perturbation Hamiltonian may be written $\Delta \hat{H}(t) \equiv \Delta \hat{H}_{13}(t) + \Delta \hat{H}_{24}(t)$ where
\[ \begin{align*}
\Delta \hat{H}_{13}(t) &= \Delta \hat{H}_1(t) + \Delta \hat{H}_3(t) \\
\Delta \hat{H}_{24}(t) &= \Delta \hat{H}_2(t) + \Delta \hat{H}_4(t)
\end{align*} \] (B.51)
with
\[ \begin{align*}
\Delta \hat{H}_1(t) &\equiv -g \int dr \left[ (2\Phi^*\tilde{n} + \Phi\tilde{m}^*) \hat{\eta} + (2\Phi\tilde{n} + \Phi^*\tilde{m}) \hat{\eta}^\dagger \right] \\
\Delta \hat{H}_2(t) &\equiv -\frac{g}{2} \int dr \left( 4\tilde{m}\tilde{\eta}^\dagger \hat{\eta} + \tilde{m}^*\tilde{\eta} \hat{\eta}^\dagger \tilde{\eta}^\dagger \right) \\
\Delta \hat{H}_3(t) &\equiv g \int dr \left( \Phi^*\tilde{n}^\dagger \hat{\eta} + \Phi\tilde{n}^\dagger \hat{\eta} \right) \\
\Delta \hat{H}_4(t) &\equiv \frac{g}{2} \int dr \tilde{\eta}^\dagger \tilde{\eta} \tilde{\eta} \tilde{\eta}.
\end{align*} \] (B.52)

Now it can be shown that
\[
\begin{align*}
\left[ \hat{H}_{HFB_1}(t), \Delta \hat{H}_{13}(t) \right] &= g \int dr \left\{ 2\Phi^* \left( \tilde{n} - \tilde{n}^\dagger \hat{\eta} \right) \left( \hat{\hbar} + g \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi + g\tilde{m}\Phi^* \right. \\
&\quad + \Phi \left( \tilde{m}^* - \tilde{\eta}^\dagger \tilde{\eta} \right) \left( \hat{\hbar} + g \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi + g\tilde{m}\Phi^* \right\} \\
&\quad -2\Phi \left( \tilde{n} - \tilde{n}^\dagger \hat{\eta} \right) \left( \hat{\hbar} + g \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi^* + g\tilde{m}\Phi \right\} \\
&\quad -\Phi^* \left( \tilde{m} - \tilde{\eta} \hat{\eta} \right) \left( \hat{\hbar} + g \left( |\Phi|^2 + 2\tilde{n} \right) \right) \Phi^* + g\tilde{m}\Phi \right\}
\end{align*}
\]

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and that
\[
\left[ \hat{H}_{HFB_2}(t), \Delta \hat{H}_{24}(t) \right] = \frac{g}{4} \int dr \left\{ \hat{\eta}^\dagger \hat{\eta}^\dagger \hat{h} \hat{\eta} + \hat{\eta}^\dagger \hat{\eta}^\dagger \left( \hat{h} \hat{\eta} + \hat{\eta}^\dagger \hat{h} \right) \hat{\eta} \right\}
\]
\[
- \left( \hat{h}^* \hat{\eta}^\dagger \right) \hat{\eta}^\dagger \hat{\eta} - 4 \hat{\eta}^\dagger \hat{h} \hat{\eta} + 4 \hat{\eta} \left( \hat{h}^* \hat{\eta}^\dagger \right) \hat{\eta}
\]
\[
- \hat{m}^* \hat{h} \hat{\eta} - \hat{m}^* \left( \hat{h} \hat{\eta} + \hat{\eta}^\dagger \hat{h} \hat{\eta}^\dagger + \hat{h}^* \hat{\eta}^\dagger \right) \hat{\eta} \}
\]
and since \( \left\langle \left[ \hat{H}_{HFB_2}(t), \Delta \hat{H}_{13}(t) \right] \right\rangle = \left\langle \left[ \hat{H}_{HFB_1}(t), \Delta \hat{H}_{24}(t) \right] \right\rangle = 0 \) by Wick’s Theorem for
ensemble averages for odd numbers of operators, we find that
\[
\left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{13}(t) \right] \right\rangle = \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{24}(t) \right] \right\rangle = 0. \quad (B.53)
\]
Hence
\[
\left\langle i \frac{d \hat{H}_{HFB}(t)}{dt} \right\rangle = \left\langle \left[ \hat{H}_{HFB}(t), \hat{H}(t) \right] \right\rangle = \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{13}(t) \right] \right\rangle + \left\langle \left[ \hat{H}_{HFB}(t), \Delta \hat{H}_{24}(t) \right] \right\rangle = 0. \quad (B.54)
\]
Therefore (B.49) holds, showing that energy is conserved in the case where the external (trapping) potential is time-independent.

**Alternative Proof of Conservation of Energy**

We now present a direct proof, which will enable us to show that Popov, G1 and G2 all violate energy conservation.

From by (2.57) we can write
\[
E_{HFB} = \left\langle \hat{H}_{HFB}(t) \right\rangle = \left\langle \hat{H}_{HFB_0}(t) \right\rangle + \left\langle \hat{H}_{HFB_1}(t) \right\rangle + \left\langle \hat{H}_{HFB_2}(t) \right\rangle
\]
where by equations (4.32) and (4.33)
\[
\left\langle \hat{H}_{HFB_0}(t) \right\rangle = \int dr \left( \Phi^* \left( \hat{h} - \mu + \frac{g}{2} |\Phi|^2 \right) \Phi - g \left( \hat{n}^2 + \frac{1}{2} |\hat{m}|^2 \right) \right)
\]
\[
\left\langle \hat{H}_{HFB_1}(t) \right\rangle = 0
\]
\[
\left\langle \hat{H}_{HFB_2}(t) \right\rangle = \int dr \left\langle \hat{\eta}^\dagger \left( \hat{h} - \mu \right) \hat{\eta} \right\rangle + \frac{g}{2} \int dr \left( 2 \left( |\Phi|^2 + 2 \hat{n} \right) \hat{n} + (\Phi^2 + \hat{m}) \hat{m}^* + \left( \Phi^{2*} + \hat{m}^* \right) \hat{m} \right)
\]
and therefore
\[
E_{HFB} = \int dr \left[ \Phi^* \left( \hat{h} - \mu \right) \Phi + \left\langle \hat{\eta}^\dagger \left( \hat{h} - \mu \right) \hat{\eta} \right\rangle + \frac{g}{2} \left( |\Phi|^4 + 2 \left( |\Phi|^2 + 2 \hat{n} \right) \hat{n} + \Phi^2 \hat{m}^* + \Phi^{2*} \hat{m} + 2 |\hat{m}|^2 \right) \right]
\]
so
\[
i \hbar \frac{d}{dt} E_{HFB} = \int dr \left\{ \left( \frac{\partial}{\partial t} \Phi^* \right) \left[ \left( \hat{h} - \mu + g \left( |\Phi|^2 + 2 \hat{n} \right) \right) \Phi + g \hat{m} \Phi^* \right]
\]
\[
+ \left[ \left( \hat{h}^* - \mu + g \left( |\Phi|^2 + 2 \hat{n} \right) \right) \Phi^* + g \hat{m}^* \Phi \right] \left( \frac{\partial}{\partial t} \Phi \right)
\]
\[
+ \left\langle i \hbar \frac{\partial}{\partial t} \hat{\eta}^\dagger \right\rangle \left( \hat{h} - \mu + g \left( |\Phi|^2 + 2 \hat{n} \right) \right) \hat{\eta} + g \left( \Phi^2 + \hat{m} \right) \hat{\eta}^\dagger \right\rangle
\]
\[
+ \left\langle i \hbar \frac{\partial}{\partial t} \hat{\eta} \right\rangle \left( \hat{h}^* - \mu + g \left( |\Phi|^2 + 2 \hat{n} \right) \right) \hat{\eta}^\dagger + g \left( \Phi^{2*} + \hat{m}^* \right) \hat{\eta} \left( i \hbar \frac{\partial}{\partial t} \hat{\eta} \right) \}
\]

(B.56)
Appendix B. Conservation Laws for HFB and Orthogonal HFB

and therefore by the GGPE (4.3) and the BdGEs (4.4), and their Hermitian conjugates, we find that
\[
\frac{i\hbar}{dt} E_{\text{HFB}} = \int dr \left[ |i\hbar \frac{\partial \Phi}{\partial t}|^2 - |i\hbar \frac{\partial \Phi}{\partial t}|^2 + \left\langle \left( i\hbar \frac{\partial \tilde{\eta}^\dagger}{\partial t} \right) \left( i\hbar \frac{\partial \tilde{\eta}}{\partial t} \right) \right\rangle - \left\langle \left( i\hbar \frac{\partial \tilde{\eta}^\dagger}{\partial t} \right) \left( i\hbar \frac{\partial \tilde{\eta}}{\partial t} \right) \right\rangle \right] = 0,
\]
\[(B.57)\]
thus we have shown that energy is conserved for standard HFB.

**Violation of energy conservation for Popov, G1 and G2**

The GGPE and BdGEs for Popov, G1 and G2 can be written in the form given by equations (B.35) - (B.37). Hence we obtain the expression
\[
\frac{i\hbar}{dt} E_{\text{HFB}} = g \int dr \left\{ \frac{\tilde{m}^* \tilde{n}}{\Phi^*} + (a - 1) \tilde{m}^* \Phi \right\} \left( i\hbar \frac{\partial \Phi}{\partial t} \right) + \left\langle \left( \frac{i\hbar}{\partial t} \right) \left( \frac{i\hbar}{\partial t} \right) \right\rangle + \text{h.c.}
\]
\[(B.58)\]
for the rate of change of energy. For Popov \(a = b = 0\), for G1 \(a = 1, b = 0\), and for G2 \(a = b = 1\), so we have
\[
\frac{i\hbar}{dt} E_{\text{HFB}} = -g \int dr \left\{ \tilde{m}^* \Phi \left( i\hbar \frac{\partial \Phi}{\partial t} \right) + \left\langle \left( \frac{i\hbar}{\partial t} \right) \left( \frac{i\hbar}{\partial t} \right) \right\rangle + \text{h.c.} \right\}
\]
\[(B.59)\]
for Popov,
\[
\frac{i\hbar}{dt} E_{\text{HFB}} = g \int dr \left\{ \left( \frac{i\hbar}{\partial t} \right) \left( \frac{i\hbar}{\partial t} \right) \right\} + \text{h.c.}
\]
\[(B.60)\]
for G1, and
\[
\frac{i\hbar}{dt} E_{\text{HFB}} = g \int dr \left\{ \tilde{m}^* \Phi \left( i\hbar \frac{\partial \Phi}{\partial t} \right) + \left\langle \left( \frac{i\hbar}{\partial t} \right) \left( \frac{i\hbar}{\partial t} \right) \right\rangle + \text{h.c.} \right\}
\]
\[(B.61)\]
for G2, so energy conservation is violated in all three cases.

**B.2.3 Conservation of Angular Momentum**

We show that the expectation value of the angular momentum \(\hat{L}\) of the BEC is conserved in a spherically symmetric harmonic trap. The rate of change of \(L\) is given by
\[
\frac{d}{dt} \langle \hat{L} \rangle = \frac{d}{dt} \left\langle \int dr \hat{\psi}^\dagger(r, t) \hat{L} \hat{\psi}(r, t) \right\rangle
\]
\[(B.62)\]
where \(\hat{L} = i\hbar (\mathbf{r} \times \nabla)\) is the angular momentum operator, and since \(\hat{\psi}(r, t) = \Phi(r, t) + \tilde{\eta}(r, t)\) by (2.30), we find that
\[
\frac{d}{dt} \langle \hat{L} \rangle = \frac{1}{i\hbar} \left\langle \int dr \left[ \left( i\hbar \frac{\partial \Phi^*}{\partial t} \right) \hat{L} \Phi + \Phi^* \hat{L} \left( i\hbar \frac{\partial \Phi}{\partial t} \right) + \left( i\hbar \frac{\partial \tilde{\eta}^\dagger}{\partial t} \right) \hat{L} \tilde{\eta} + \tilde{\eta}^\dagger \hat{L} \left( i\hbar \frac{\partial \tilde{\eta}}{\partial t} \right) \right] \right\rangle
\]
where $i\hbar \frac{\partial}{\partial t} \Phi$ and $i\hbar \frac{\partial}{\partial t} \eta$ are given by the time-dependent GGPE (4.3), and the BdGEs (4.4) and their respective complex conjugates. Using the equations (B.19) and (B.20) with $\hat{D} \equiv \hat{L}$, i.e.

$$\int dr \left( -\hat{h}_\Omega^*(r) \phi(r,t) \right) \left( \hat{L}(r) \psi(r,t) \right) + \phi(r,t) \hat{L}(r) \left( \hat{h}_\Omega(r) \psi(r,t) \right) = \int dr \psi(r,t) \phi(r,t) \hat{L}(r) V_T(r)$$

and

$$\left\langle \int dr \left( -\hat{h}_\Omega^*(r) \eta^+(r,t) \right) \left( \hat{L}(r) \eta(r,t) \right) + \eta^+(r,t) \hat{L}(r) \left( \hat{h}_\Omega(r) \eta(r,t) \right) \right\rangle = \int dr \eta(r,t) \hat{L}(r) V_T(r),$$

we obtain

$$\frac{d}{dt} \langle L \rangle = \frac{1}{i\hbar} \int dr \left[ |\Phi|^2 \hat{L} V_T + |\Phi|^2 \hat{L} \left( |\Phi|^2 + 2\tilde{n} \right) - \frac{i}{2} g \tilde{m}^* \hat{L} \left( \Phi^2 \right) - \frac{i}{2} g \tilde{m} \hat{L} \left( \Phi^2 \right) \right]$$

$$+ \tilde{n} \hat{L} V_T + 2\tilde{n} \hat{L} \left( |\Phi|^2 + \tilde{n} \right) - \frac{1}{2} g \left( \Phi^2 + \tilde{m}^* \right) \hat{L} \tilde{m} - \frac{1}{2} g \left( \Phi^2 + \tilde{m} \right) \hat{L} \tilde{m}^*.$$}

This can be rewritten as

$$\frac{d}{dt} \langle L \rangle = \frac{1}{i\hbar} \int dr \left[ \left( |\Phi|^2 + \tilde{n} \right) \hat{L} V_T + g \hat{L} \left( |\Phi|^2 + \tilde{n} \right)^2 \right]$$

$$- \frac{g}{2} \hat{L} \left( \tilde{m}^* \Phi^2 \right) - \frac{g}{2} \hat{L} \left( \tilde{m} \Phi^2 \right) - \frac{g}{2} \hat{L} \left( |\tilde{m}|^2 \right) .$$

Hence using equation (B.6)

$$\frac{d}{dt} \langle L \rangle = \frac{1}{i\hbar} \int dr \left( |\Phi|^2 + \tilde{n} \right) \hat{L} V_T .$$

The conservation of angular momentum therefore depends entirely on the trapping potential. Angular momentum is conserved whenever $\hat{L} V_T = 0$. This is clearly the case whenever spherical symmetry exists. Thus we see that in a spherically symmetric harmonic trap ($\hat{L} V_T = 0$)

$$\frac{d}{dt} \langle L \rangle = 0$$

(B.64)

showing that angular momentum is conserved. In an axially symmetric harmonic trap, $\hat{L}_z V_T = 0$

$$\frac{d}{dt} \langle L_z \rangle = 0$$

(B.65)

so the z-component of the angular momentum is conserved. Clearly the angular momentum is always conserved in the absence of any trapping potential ($V_T = 0$).

This result also holds for any linear differential operator $\hat{D}$, i.e. $\frac{d}{dt} \hat{D} = \frac{1}{i\hbar} \int dr \left( |\Phi|^2 + \tilde{n} \right) \hat{D} V_T$, therefore the same result holds for linear momentum.
Violation of angular momentum conservation for Popov, G1 and G2

We show that the expectation value of the angular momentum $\hat{L}$ of the BEC is violated whether a trapping potential is present or not.

The GGPE and BdGEs for Popov, G1 and G2 can be written in the form given by equations (B.35) - (B.37). Hence we obtain the expression

$$\frac{d\langle L \rangle}{dt} = \int d\mathbf{r} \left[ (|\Phi|^2 + \tilde{n}) \hat{L} V_T \right] + I_R \tag{B.66}$$

where

$$I_R = \frac{2g}{\hbar} \text{Re} \left\{ \frac{1}{i} \int d\mathbf{r} \left[ -(a - 1)\tilde{m}^* \Phi L(\Phi) - 2b\tilde{m}^* \frac{\tilde{n} \Phi}{|\Phi|^2} L(\Phi) - 2\tilde{m}^* \frac{(a |\Phi|^2 + b\tilde{n})}{\Phi^*} \right] \right\} \tag{B.67}$$

For Popov $a = b = 0$, for G1 $a = 1, b = 0$, and for G2 $a = b = 1$, so we have

$$I_R = \frac{2g}{\hbar} \text{Re} \left\{ \frac{1}{i} \int d\mathbf{r} \left[ \tilde{m}^* \Phi \hat{L}(\Phi) \right] \right\} \tag{B.68}$$

for Popov,

$$I_R = -\frac{4g}{\hbar} \text{Re} \left\{ \frac{1}{i} \int d\mathbf{r} \left[ \tilde{m}^* |\Phi|^2 \hat{L}(\Phi) \right] \right\} \tag{B.69}$$

for G1, and

$$I_R = -\frac{4g}{\hbar} \text{Re} \left\{ \frac{1}{i} \int d\mathbf{r} \left[ \tilde{m}^* \frac{\tilde{n} \Phi}{|\Phi|^2} \hat{L}(\Phi) + \tilde{m}^* \left( |\Phi|^2 + \tilde{n} \right) \frac{\tilde{m} \Phi^*}{\Phi^*} \right] \right\} \tag{B.70}$$

for G2. In general, $I_R \neq 0$, so angular momentum conservation is violated in all three cases, regardless of the trapping potential.

B.3 Conservation Laws for Orthogonal HFB

B.3.1 Particle Conservation

Since

$$\int d\mathbf{r} d\mathbf{r}' \Phi^*(\mathbf{r}, t) \hat{P}(\mathbf{r}, \mathbf{r}', t) \phi(\mathbf{r}', t) = \int d\mathbf{r} d\mathbf{r}' \Phi(\mathbf{r}, t) \hat{P}^*(\mathbf{r}, \mathbf{r}', t) \phi^*(\mathbf{r}', t) = 0$$

by the orthogonality relation (4.77), we obtain for the modified GGPE (4.102) in the rotating frame (or alternatively in the LAB or in the translating frame)

$$\frac{dN_c(t)}{dt} = \frac{g}{\hbar} \int d\mathbf{r} \left( \tilde{m}(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) - \tilde{m}^*(\mathbf{r}, t) \Phi^2(\mathbf{r}, t) \right)$$
Appendix B. Conservation Laws for HFB and Orthogonal HFB

as before. For the modified BdGEs (4.103), we have

\[
\frac{id}{dt} \int dr |u_q(r, t)|^2 = \frac{g}{\hbar} \int dr dr' \left[ Q(r, r', t) (\Phi^2(r', t) + \tilde{m}(r', t)) u_q(r, t) - Q^*(r, r', t) \left( \Phi^* r'(r', t) + \tilde{m}^*(r', t) \right) v_q(r', t) u_q^*(r, t) \right]
\]

where by (4.79) \(Q(r, r') = \delta(r - r') - \phi(r, t)\phi^*(r', t)\). Now

\[
\int dr \Phi(r, t) u_q^*(r, t) = \int dr \Phi^*(r, t) u_q(r, t) = 0
\]

by orthogonality condition (4.77), we find that

\[
\frac{id}{dt} \int dr |u_q|^2 = \frac{g}{\hbar} \int dr \left( (\Phi^2 + \tilde{m}) v_q u_q^* - (\Phi^* r + \tilde{m}^*) u_q v_q^* \right)
\]

as before. Similarly

\[
\frac{i\hbar}{dt} \int dr |v_q|^2 = \frac{g}{\hbar} \int dr \left( (\Phi^2 + \tilde{m}) v_q u_q^* - (\Phi^* r + \tilde{m}^*) u_q v_q^* \right).
\]

Therefore we obtain, as we did previously

\[
\frac{d\tilde{N}(t)}{dt} = i \frac{g}{\hbar} \int dr \left( \tilde{m}^*(r, t)\Phi^2(r, t) - \tilde{m}(r, t)\Phi^* r(t) \right) = -\frac{dN_c(t)}{dt}
\]

showing that particles are conserved for time-dependent orthogonal HFB.

B.3.2 Conservation of Angular Momentum

We show that the expectation value of the angular momentum \(\hat{L}\) of the BEC is conserved in a spherically symmetric harmonic trap.

The rate of change of \(L\) is given by (B.62)

\[
\frac{d}{dt} \left< \hat{L} \right> = \frac{d}{dt} \left< \int dr \hat{\psi}^\dagger(r, t) \hat{L} \hat{\psi}(r, t) \right>
\]

where \(\hat{L} = i\hbar(\mathbf{r} \times \nabla)\) is the angular momentum operator, and since \(\hat{\psi}(r, t) = \hat{\Phi}(r, t) + \hat{\eta}(r, t)\) by (4.72), we find that

\[
\frac{d}{dt} \left< \hat{L} \right> = \frac{1}{i\hbar} \left< \int dr \left[ \left( i\hbar \frac{\partial \hat{\Phi}^\dagger}{\partial t} \right) \hat{L} \hat{\Phi} + \hat{\Phi}^\dagger \hat{L} \left( i\hbar \frac{\partial \hat{\Phi}}{\partial t} \right) + \left( i\hbar \frac{\partial \hat{\eta}^\dagger}{\partial t} \right) \hat{L} \hat{\eta} + \hat{\eta}^\dagger \hat{L} \left( i\hbar \frac{\partial \hat{\eta}}{\partial t} \right) \right] \right>
\]

Hence by the modified GGPE (4.93) for the condensate operator \(\hat{\Phi}\), and the orthogonal BdGEs (4.103), and their respective complex conjugates, applying the orthogonality condition (4.77) \(\int dr \phi^*(r, t)\eta(r, t) = 0\) and its complex conjugate \(\int dr \phi(r, t)\eta^\dagger(r, t) = 0\), and
from the definition (4.73) for the condensate operator \( \hat{\Phi}(r, t) \equiv \phi(r, t)\hat{\alpha}_c(t) \), and from the result for standard HFB, we obtain (after some re-arranging)

\[
\frac{d}{dt} \langle L \rangle = \int dr \left( n_c + \bar{n} \right) \hat{L} V_T + \left\langle \int dr \left\{ \left[ -\hat{A}^\dagger + \sqrt{N_c} \hat{\eta}^\dagger \eta \right] \int dr' \left( \hat{\eta}(r', t) \hat{L}^* \eta^*(r', t) + \hat{\eta}^*(r', t) \hat{L} \eta(r', t) \right) \phi^*(r', t) \right\} \right\rangle \hat{L} \Phi \\
+ \left[ -\hat{A} + \frac{1}{\sqrt{N_c}} \int dr' \left( \hat{\eta}^\dagger(r', t) \hat{L} \eta(r', t) + \hat{\eta}(r', t) \hat{L}^* \eta^*(r', t) \right) \phi(r', t) \right] \hat{\eta}(r, t) \hat{L} \Phi^* \rangle
\]

So

\[
\frac{dL}{dt} = \int dr \left( |\Phi|^2 + \bar{n} \right) \hat{L} V_T
\]

provided

\[
\hat{A}(r, t) = -\frac{1}{\sqrt{N_c}} \int dr' \left( \hat{\eta}^\dagger(r', t) \hat{L} \eta(r', t) + \hat{\eta}(r', t) \hat{L}^* \eta^*(r', t) \right) \phi(r', t) \hat{\eta}(r, t).
\]

### B.3.3 Calculation of the Precessional Frequency of Off-axis Vortices in Quasi-2D BECs in the Orthogonal Formalism

From the time-independent continuity equation for the condensate (4.113)

\[
\frac{\hbar^2}{2m} \left( \Phi(r) \nabla^2 \Phi^*(r) - \Phi^*(r) \nabla^2 \Phi(r) \right) + i\hbar \Omega \cdot (r \times \nabla) |\Phi(r)|^2 + C(r) = 0
\]

where

\[
C(r) \equiv g \left( \bar{m}(r) \Phi^2(r) - \bar{m}^*(r) \Phi^*(r) \right) + G^*(r) - G(r)
\]

and

\[
G(r) \equiv \Phi^*(r) \int dr' \hat{P}(r', r) \phi(r')
\]

for the orthogonal formalism, we find for the 2D system in polar coordinates that

\[
\hbar \Omega r^2 \left( R_{\theta\theta}^{2R} + I_{\theta\theta}^{2I} \right) = \frac{\hbar^2}{2m} \left[ r^2 \left( \frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial \theta^2} \right) \right] + r \left( R_{\theta r}^{2I} - I_{\theta r}^{2R} \right) + \left( R_{\theta\theta}^{2R} - I_{\theta\theta}^{2I} \right)
\]

Multiplying both sides by \( (R_{\theta\theta}^{2R} + I_{\theta\theta}^{2I}) \) where \( R \equiv \text{Re} \{ \Phi \} \) and \( I \equiv \text{Im} \{ \Phi \} \), and integrating over all space, we find that

\[
\Omega = \frac{\int_0^{2\pi} \int_0^\infty A(r, \theta) B(r, \theta) r dr d\theta}{\int_0^{2\pi} \int_0^\infty (A(r, \theta))^2 r dr d\theta}
\]

where we have defined

\[
A(r, \theta) \equiv r^2 \left( R_{\theta r}^{2R} + I_{\theta r}^{2I} \right)
\]
and
\[
B(r, \theta) \equiv \frac{\hbar}{2m} \left[ r^2 \left( R \frac{\partial^2 I}{\partial r^2} - I \frac{\partial^2 R}{\partial r^2} \right) + r \left( R \frac{\partial I}{\partial r} - I \frac{\partial R}{\partial r} \right) + \left( R \frac{\partial^2 I}{\partial \theta^2} - I \frac{\partial^2 R}{\partial \theta^2} \right) \right] + \frac{r^2}{2\hbar} C(r, \theta)
\]
(B.77)

where
\[
C(r, \theta) \equiv g \left( \tilde{m}(r, \theta) \Phi^2(r, \theta) - \tilde{m}^*(r, \theta) \Phi^2(r, \theta) \right) + G^*(r, \theta) - G(r, \theta)
\]
(B.78)

and
\[
G(r, \theta) \equiv \Phi^*(r, \theta) \int_0^{2\pi} \int_0^{\infty} r' dr' d\theta' \tilde{P}(r', \theta', r, \theta) \phi(r', \theta')
\]
(B.79)

with
\[
\tilde{P}(r', \theta', r, \theta) = \left( \tilde{n}(r', \theta', r, \theta) \hat{L}(r', \theta') + \tilde{m}(r', \theta', r, \theta) \hat{M}^*(r', \theta') \right) / \sqrt{N_c}
\]
(B.80)
Appendix C

Solution of the Time-independent and Time-dependent HFB Equations

C.1 Single-particle Basis Functions for BECs having Axially-symmetric Trap Confinement

C.1.1 Axially Symmetric System in Cylindrical Coordinates

We first consider the case where there are no inter-atomic interactions, i.e. $U = 0$. Then the GGPE becomes

$$\hat{h}(r)\Phi^{(0)}(r) = \mu^{(0)}\Phi^{(0)}(r) \quad (C.1)$$

where $\Phi^{(0)}(r)$ is the single particle wave-function. Consider [170]

$$\Phi^{(0)}(r) = R(r)Z(z)e^{imb}\sqrt{2\pi} \quad (C.2)$$

Substituting this into the single-particle Schrödinger equation (C.1) gives us

$$\frac{1}{R(r)} \left[ - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{m^2}{r^2} + r^2 - \mu \right] R(r) = -\frac{1}{Z(z)} \left[ - \frac{d^2}{dz^2} + \lambda^2 z^2 \right] Z(z) = -\Lambda \quad (C.3)$$

where $\Lambda$ is a constant. Hence we get

$$\left[ - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{m^2}{r^2} + r^2 - (\mu_r - \Lambda) \right] R(r) = 0 \quad (C.4)$$

for the radial equation, and

$$\left[ - \frac{d^2}{dz^2} + \lambda^2 z^2 - \Lambda \right] Z(z) = 0 \quad (C.5)$$

for the axial equation.
C.1.2 The Axial Equation

Let $\xi = \lambda^{1/2} z$, then

\[
-\frac{d^2}{d\xi^2} + \xi^2 - \Lambda' \right] Z(\xi) = 0 \quad (C.6)
\]

where $\Lambda' = \Lambda / \lambda$. This is just the harmonic oscillator equation with eigenstates $Z_k(\xi) = (1/\sqrt{2^n n!})^{1/2} \exp(-\xi^2/2)H_k(\xi)$, where $H_k(\xi)$ is a Hermite polynomial, and eigenvalues $\Lambda'_k = 2k + 1$. Therefore the eigenstates for the axial equation are given by

\[
Z_k(z) = N_k \exp(-\lambda z^2/2)H_k(\lambda^{1/2} z) \quad (C.7)
\]

and the eigenvalues by

\[
\Lambda_k = \lambda (2k + 1) \quad (C.8)
\]

where

\[
N_k = \left( \frac{\lambda^{1/2}}{\sqrt{\pi 2^k k!}} \right)^{1/2} \quad (C.9)
\]

\[
\left[ -\frac{d^2}{dz^2} + \lambda^2 z^2 - \lambda (2k + 1) \right] Z_k(z) = 0. \quad (C.10)
\]

C.1.3 The Radial Equation

By equation (C.4), the radial equation may be written

\[
\left[ - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{m^2}{r^2} + r^2 - \mu \right] R(r) = 0 \quad (C.11)
\]

where

\[
\mu = (\mu_r - \lambda (2k + 1)) \quad (C.12)
\]

Let

\[
R(r) = e^{-r^2/2}r^{|m|} F(r) \quad (C.13)
\]

and substitute into the radial equation (C.11), to get

\[
\frac{d^2 F}{dr^2} + \left[ \frac{2|m| + 1}{r} - 2r \right] \frac{dF}{dr} + \left[ \mu - 2(|m| + 1) \right] F = 0
\]

Let $\rho = r^2$, and substitute into the above, this gives

\[
\rho \frac{d^2 F}{d\rho^2} + [|m| + 1 - \rho] \frac{dF}{d\rho} - \frac{1}{2} \left[ (|m| + 1) - \frac{1}{2} \mu \right] F = 0
\]
In order to render the solution physical, we require that the quantity \(-\frac{1}{2} \left( |m| + 1 \right) - \frac{1}{2} \mu\) be an integer, \(n\), say, i.e.

\[
n = -\frac{1}{2} \left( |m| + 1 \right) - \frac{1}{2} \mu.
\]

Then

\[
\rho \frac{d^2 F}{d \rho^2} + |m| + 1 - \rho \frac{d F}{d \rho} + n F = 0
\]

which is in the form of the associated Laguerre differential equation, so we may write

\[
F(\rho) = N_n^{m|} L_n^{m|}(\rho)
\]

where \(L_n^{m|}(\rho)\) is an associated Laguerre polynomial. Hence the radial equation has eigenstates given by

\[
R_n^{m|}(r) = N_n^{m|} e^{-r^2/2} r^{m|} L_n^{m|}(r^2)
\]

with eigenvalues

\[
\mu = 2 \left( 2n + 1 + |m| \right)
\]

where

\[
N_n^{m|} = \left( \frac{2n!}{(n + |m|)!} \right)^{1/2}
\]

is the normalisation constant, i.e.

\[
\left[ - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + \frac{m^2}{r^2} + r^2 - 2 \left( 2n + 1 + |m| \right) \right] R_n^{m|}(r) = 0.
\]

The chemical potential \(\mu_r\) is given by

\[
\mu_r = 2 \left( 2n + 1 + |m| \right) + \lambda \left( 2k + 1 \right).
\]

### C.1.4 Single Particle Eigenstates

The single particle eigenstates may therefore be written as

\[
\Phi_{nkm}^{(0)}(r) = R_n^{m|}(r) Z_k(z) e^{im\theta} \sqrt{2\pi}
\]

with eigenvalue

\[
\mu_{nkm} = 2 \left( 2n + 1 + |m| \right) + \lambda \left( 2k + 1 \right).
\]

Alternatively, defining the Laguerre basis functions

\[
\xi_{mn}(r, \theta) = \left( \frac{n!}{\pi (n + |m|)!} \right)^{1/2} e^{im\theta} e^{-r^2/2} r^{m|} L_n^{m|}(r^2) = \frac{e^{im\theta}}{\sqrt{2\pi}} R_n^{m|}(r)
\]

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we may also write the single particle eigenstates in the form

\[ \Phi^{(0)}_{nkm}(r) = \xi_{mn}(r, \theta)Z_k(z). \]  

(C.22)

The motivation for defining the Laguerre basis functions \( \{\xi_{m,n}(r, \theta)\} \) is that they form an orthonormal set, i.e.

\[ \int_0^{2\pi} \int_0^{\infty} r dr d\theta \xi_{mn}^*(r, \theta) \xi_{m'n'}(r, \theta) = \delta_{n,n'}\delta_{m,m'} \]  

(C.23)

whereas the functions \( \{R_{n|m}(r)\} \) are only orthogonal for a given value of the quantum number \( m \), i.e.

\[ \int_0^{\infty} r dr R_{n|m}(r)R_{n'|m'}(r) = \delta_{n,n'} \]  

(C.24)

but

\[ \int_0^{\infty} r dr R_{n|m}(r)R_{n'|m'}(r) \neq \delta_{n,n'}\delta_{m,m'}. \]  

(C.25)

### C.1.5 The Hermite and Laguerre Basis Functions

#### The Hermite Basis Set

We use the notation \( \zeta_k(z) \equiv Z_k(z) \) for the set of eigenstates satisfying (C.6) and refer to the set of basis functions \( \{\zeta_k(z), k = 0, \ldots, K\} \) as the Hermite single particle basis corresponding to a computational mode cut-off of \( k = 0, \ldots, K \).

#### The Laguerre Basis Set

We use the notation \( \xi_{ln}(r) \equiv R_{n|l}(r) \) to represent the radial Laguerre function with principle quantum number \( n \), and angular quantum number \( l \) satisfying the the radial equation (C.17), and rewrite \( \xi_{ln}(r, \theta) \) given by (C.21) in the form

\[ \xi_{ln}(r, \theta) = \frac{e^{il\theta}}{\sqrt{2\pi}} \xi_{ln}(r), \]  

(C.26)

where

\[ \xi_{ln}(r) = \left( \frac{2n!}{(n+|l|)!} \right)^{1/2} e^{-r^2/2} r^{|l|} L_n^{(|l|)}(r^2). \]  

(C.27)

We refer to the set of basis functions

\[ \{ \xi_{ln}(r, \theta), \ n = 0, \ldots, N, \ l = 0, \pm 1, \ldots, \pm L \} \]
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as the Laguerre single particle basis corresponding to a computational mode cut-off of \( n = 0, \ldots, N \) and \( l = 0, \pm 1, \ldots, \pm L \). In the 2D case where the axial confinement is sufficiently strong that we can neglect all axial states other than the lowest energy state, i.e., we can restrict ourselves to \( k = 0 \), we integrate out the axial coordinate \( z \). We generally absorb the energy term of \( \lambda \) harmonic energy units \( \hbar \omega r/2 \) in the expression \( \mu_{n0l} = 2 (2n + 1 + |l|) + \lambda \) into the system chemical potential \( \mu \) and write the single particle eigenvalue energies corresponding to the Laguerre basis functions as \( \mu^{(SP)}_{ln} = 2 (2n + 1 + |l|) \).

C.2 Time-independent HFB Equations

C.2.1 General Method of Solution for BECs in Axially Symmetric Harmonic Trap using Single Particle Basis Functions

We expand the condensate wave-function \( \Phi(\mathbf{r}) \) and the quasi-particle amplitudes \( u_q(\mathbf{r}) \) and \( v_q(\mathbf{r}) \) in terms of the single-particle basis functions \( \xi_k(\mathbf{r}) = \xi_{ln}(r, \theta)\zeta_k(z) \). These single-particle basis functions are solutions of the (single-particle) time-independent Schrödinger equation with respective energy eigenvalues \( \mu^{(SP)}_k \), viz.

\[
\mu^{(SP)}_k \xi_k(\mathbf{r}) = \hat{h}(\mathbf{r})\xi_k(\mathbf{r}).
\]  

(C.28)

Thus we may write the condensate wave function \( \Phi(\mathbf{r}) \) as

\[
\Phi(\mathbf{r}) = \sum_k a_{0k} \xi_k(\mathbf{r})
\]  

(C.29)

and the quasiparticle amplitudes \( u_q(\mathbf{r}) \) and \( v_q(\mathbf{r}) \) as

\[
u_q(\mathbf{r}) = \sum_k d_{qk} \xi_k(\mathbf{r})
\]  

and

\[
v_q(\mathbf{r}) = \sum_k d_{qk} \xi_k(\mathbf{r})
\]  

(C.31)

respectively. We substitute (C.29) into the dimensionless modified GGPE (5.20), i.e.

\[
\mu \Phi(\mathbf{r}) = \left( \hat{h}(\mathbf{r}) + C_{3D} \left( |\Phi(\mathbf{r})|^2 + 2\tilde{n}(\mathbf{r}) \right) \right) \Phi(\mathbf{r}) + C_{3D} \tilde{m}(\mathbf{r}) \Phi^*(\mathbf{r}) - \int d\mathbf{r}' \tilde{P}(\mathbf{r}', \mathbf{r}) \Phi(\mathbf{r}')
\]  

(C.32)

where we have neglected \( \Delta \mu \), which we showed to be negligible in Chapter 4. In this way we obtain the matrix (eigenvalue) equation for the coefficients \( a_k \) for the condensate
wave-function $\Phi(r)$ given by
\[
\mu a_k = \sum_{k'} (A_{k,k'} + B_{k,k'}) a_{k'}
\] (C.33)
written in terms of the matrix elements
\[
A_{k,k'} \equiv \mu_{k,\Omega}^{(SP)} \delta_{k,k'} + C_{3D} \int dr \xi_k^*(r) \left( |\Phi(r)|^2 + 2\bar{n}(r) \right) \xi_{k'}(r) - P_{k,k'}
\] (C.34)
and
\[
B_{k,k'} \equiv C_{3D} \int dr \xi_k^*(r) \bar{m}(r) \xi_{k'}(r)
\] (C.35)
where
\[
P_{k,k'} = \int dr dr' \xi_k^*(r) \left[ \bar{n}(r',r) \left( \mu_{k',\Omega}^{(SP)} - \mu + 2C_{3D} \left( |\Phi(r')|^2 + \bar{n}(r') \right) \right) + C_{3D} \bar{m}(r',r) \left( \Phi^2(r') + \bar{m}^*(r') \right) \right] \xi_{k'}(r') / N_c.
\] (C.36)
Note that we use lowest energy eigenvector for condensate wave-function, and hence the coefficients $a_{k'}$. Similarly we substitute (C.30) and (C.31) into the dimensionless orthogonal BdGEs (5.21)
\[
\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r,r') & \mathcal{M}(r,r') \\ -\mathcal{M}^*(r,r') & -\hat{L}^*(r,r') \end{bmatrix} \begin{bmatrix} u_q(r') \\ v_q(r') \end{bmatrix}
\] (C.37)
where, as before
\[
\hat{L}(r,r') = \hat{h}(r) - \mu + 2C_{3D} \left( |\Phi(r)|^2 + \bar{n}(r) \right)
\]
\[
\mathcal{M}(r,r') = C_{3D} \left( \Phi^2(r) + \bar{m}(r) \right)
\] (C.38)
with
\[
\hat{L}(r) = \hat{h}(r) - \mu + 2C_{3D} \left( |\Phi(r)|^2 + \bar{n}(r) \right)
\]
\[
\mathcal{M}(r) = C_{3D} \left( \Phi^2(r) + \bar{m}(r) \right)
\] (C.39)
to obtain matrix (eigenvalue) equations for the coefficients $c_{qk}$ and $d_{qk}$ for the quasi-particle amplitudes $u_q(r)$ and $v_q(r)$
\[
\epsilon_q \begin{bmatrix} c_{qk} \\ d_{qk} \end{bmatrix} = \sum_{k'} \begin{bmatrix} L^{(u)}_{q,k,k'} & M^{(u)}_{q,k,k'} \\ -M^{(v)}_{q,k,k'} & -L^{(v)}_{q,k,k'} \end{bmatrix} \begin{bmatrix} c_{qk'} \\ d_{qk'} \end{bmatrix}
\] (C.40)
written in terms of the respective matrix elements
\[
L^{(u)}_{q,k,k'} = \left( \mu_{k}^{(SP)} - \mu \right) \left( \delta_{k,k'} - \frac{1}{N_c} J^{(1)}_k J^{(1)*}_{k'} \right) + I^{(u)}_{q,k,k'},
\] (C.41)
\[
L^{(v)}_{q,k,k'} = \left( \mu_{k}^{(SP)} - \mu \right) \left( \delta_{k,k'} - \frac{1}{N_c} J^{(2)}_k J^{(2)*}_{k'} \right) + I^{(v)}_{q,k,k'},
\] (C.42)
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\[ M^{(u)}_{q,k,k'} \equiv C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c} I^{(1)}_k \Phi^*(r) \right) \left( \Phi^2(r) + \bar{m}(r) \right) \xi_{k'}(r), \]  
\[ M^{(v)}_{q,k,k'} \equiv C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c} I^{(2)}_k \Phi(r) \right) \left( \Phi^{*2}(r) + \bar{m}^*(r) \right) \xi_{k'}(r), \]

where
\[ I^{(u)}_{q,k,k'} \equiv 2C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c} I^{(1)}_k \Phi^*(r) \right) \left( |\Phi(r)|^2 + \bar{n}(r) \right) \xi_{k'}(r), \]
\[ I^{(v)}_{q,k,k'} \equiv 2C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c} I^{(2)}_k \Phi(r) \right) \left( |\Phi(r)|^2 + \bar{n}(r) \right) \xi_{k'}(r), \]
\[ I^{(1)}_k \equiv \int dr \xi^*_k(r) \Phi(r), \]
\[ I^{(2)}_k \equiv \int dr \xi^*_k(r) \Phi^*(r). \]

Defining the vectors \( \mathbf{a}, \mathbf{c}_q, \) and \( \mathbf{d}_q \) corresponding to the coefficients \( a_k, c_{q,k}, \) and \( d_{q,k} \), and the matrices \( \mathbf{A}, \mathbf{B}, \mathbf{L}^{(u)}_q, \mathbf{M}^{(u)}_q, \mathbf{L}^{(v)}_q, \) and \( \mathbf{M}^{(v)}_q \) corresponding to the matrix elements \( A_{k,k'}, B_{k,k'}, L^{(u)}_{q,k,k'}, M^{(u)}_{q,k,k'}, L^{(v)}_{q,k,k'}, \) and \( M^{(v)}_{q,k,k'} \) respectively, we obtain the following matrix equations:

The coefficients for the condensate wavefunction (GGPE) and the chemical potential are obtained by solving the matrix eigenvalue equation

\[ \mu \mathbf{a} = (\mathbf{A} + \mathbf{B}) \mathbf{a}. \]  

\[ \epsilon_q \begin{bmatrix} \mathbf{c}_q \\ \mathbf{d}_q \end{bmatrix} = \begin{bmatrix} \mathbf{L}^{(u)}_q & \mathbf{M}^{(u)}_q \\ -\mathbf{M}^{(v)}_q & -\mathbf{L}^{(v)}_q \end{bmatrix} \begin{bmatrix} \mathbf{c}_q \\ \mathbf{d}_q \end{bmatrix} \]

corresponding to the BdGEs. In the laboratory (LAB) frame in the axially symmetric case and in the absence of any vortices, we have \( \mathbf{L}^{(u)}_q = \mathbf{L}^{(v)}_q \) and \( \mathbf{M}^{(u)}_q = \mathbf{M}^{(v)}_q \), but this is not the case in general.

We generally neglect the projection part \( \int dr \tilde{P}(r',r)\phi(r') \) in the time-independent solutions for the GGPE since results (not presented here) indicate that the effect is small and implies an unnecessary increase in the computational effort in solving the orthogonal HFB equations. The projection part was included in some of the solutions, the effect of its inclusion having a negligible effect on the time-independent solution. The projection part is however crucially important in the time-dependent formalism in the conservation of angular and linear momentum.
C.2.2 Solutions for Quasi-2D BEC in Axially-symmetric Trap - Axially-symmetric Solutions

In the case of axial symmetry of the solutions, we can integrate out the azimuthal coordinate θ to obtain the radial time-independent orthogonal HFB equations comprised of the radial time-independent GGPE (7.14)

\[
\mu \Phi(r) = \left( \hat{h}_m(r) - \mu + C_{2D}^R (|\Phi(r)|^2 + 2\tilde{n}(r)) \right) \Phi(r) + C_{2D}^R \tilde{m}(r) \Phi(r) - \int_0^\infty r' dr' \hat{P}(r', r) \phi(r')
\]

and the radial time-independent orthogonal BdGEs (7.15)

\[
\epsilon_{lq} \begin{bmatrix} u_{lq}(r) \\ v_{lq}(r) \end{bmatrix} = \int_0^\infty r' dr' \begin{bmatrix} Q_l(r, r') \hat{L}_{l+m}(r') & Q_l(r, r') \mathcal{M}(r') \\ -Q_l(r, r') \mathcal{M}(r') & -Q_l(r, r') \hat{L}_{l-m}(r') \end{bmatrix} \begin{bmatrix} u_{lq}(r') \\ v_{lq}(r') \end{bmatrix}
\]

(see sections 5.3.1 and 7.2). In this case we can expand the radial condensate wave-function Φ(r) and the radial quasi-particle amplitudes u_{lq}(r) and v_{lq}(r) in terms of the radial Laguerre basis functions ξ_{ln}(r), i.e.

\[
\Phi(r) = \sum_n a_n \xi_{mn}(r)
\]

for the condensate wave-function, and

\[
u_{lq}(r) = \sum_{l,n} c_{ql,n} \xi_{l+m,n}(r)
\]

and

\[
v_{lq}(r) = \sum_{l,n} d_{ql,n} \xi_{l-m,n}(r)
\]

for the quasi-particle amplitudes. Here we have allowed for the existence of an on-axis vortex of vorticity m. In the case of no vortices, m = 0. Substituting (C.53) into the GGPE (C.51), and (C.54),(C.55) into the orthogonal BdGEs (C.52), we find that

\[
\mu a_n = \sum_{n'} A_{n,n'} a_{n'}
\]

and

\[
\epsilon_{lq} \begin{bmatrix} c_{ql,n} \\ d_{ql,n} \end{bmatrix} = \sum_{n'} \begin{bmatrix} L_{l,q,n,n'}^{(u)} & M_{l,q,n,n'}^{(u)} \\ -M_{l,q,n,n'}^{(v)} & -L_{l,q,n,n'}^{(v)} \end{bmatrix} \begin{bmatrix} c_{ql,n'} \\ d_{ql,n'} \end{bmatrix}
\]

where we have defined

\[
A_{n,n'} \equiv \left( \mu_{mn}^{(SP)} - m\Omega \right) \delta_{n,n'} + C_{2D}^R \int_0^\infty r dr \xi_{mn}(r) \left( |\Phi(r)|^2 + 2\tilde{n}(r) + \tilde{m}(r) \right) \xi_{mn'}(r) - P_{n,n'}
\]

(766)
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with

\[ P_{n,n'} = \int_0^\infty \int_0^\infty r dr' dr' \xi_{mn}(r) \left[ \tilde{n}(r', r) \left( \mu_{mn}^{(SP)} - m \Omega - \mu + 2C_{2D}^R (|\Phi(r')|^2 + \tilde{n}(r')) \right) + C_{2D}^R \tilde{m}(r', r) (\Phi^2(r') + \tilde{m}(r')) \right] \xi_{mn'}(r') / N_c, \]

(C.59)

and

\[ L_{q,l,n,n'}^{(u)} = (\mu_{ln}^{(SP)} - (l + m) \Omega - \mu) \left( \delta_{l,l'} \delta_{n,n'} - \frac{\delta_{l,0}}{N_c} I_{l+m,n,n'}^{(1)} \right) + I_{q,l,n,n'}^{(u)}, \]

(C.60)

\[ L_{q,l,n,n'}^{(v)} = (\mu_{ln}^{(SP)} + (l - m) \Omega - \mu) \left( \delta_{l,l'} \delta_{n,n'} - \frac{\delta_{l,0}}{N_c} I_{l-m,n,n'}^{(2)} \right) + I_{q,l,n,n'}^{(v)}, \]

(C.61)

\[ M_{q,l,n,n'}^{(u)} = C_{2D}^R \int_0^\infty dr \left( \xi_{l+m,n}(r) - \frac{\delta_{l,0}}{N_c} I_{l+m,n}^{(1)} \Phi(r) \right) (\Phi^2(r) + \tilde{m}(r)) \xi_{l-m,n'}(r), \]

(C.62)

\[ M_{q,l,n,n'}^{(v)} = C_{2D}^R \int_0^\infty dr \left( \xi_{l-m,n}(r) - \frac{\delta_{l,0}}{N_c} I_{l-m,n}^{(2)} \Phi(r) \right) (\Phi^2(r) + \tilde{m}(r)) \xi_{l+m,n'}(r), \]

(C.63)

where

\[ I_{q,l,n,n'}^{(u)} = 2C_{2D}^R \int_0^\infty dr \left( \xi_{l+m,n}(r) - \frac{\delta_{l,0}}{N_c} I_{l+m,n}^{(1)} \Phi(r) \right) (|\Phi(r)|^2 + \tilde{n}(r)) \xi_{l+m,n'}(r), \]

(C.64)

\[ I_{q,l,n,n'}^{(v)} = 2C_{2D}^R \int_0^\infty dr \left( \xi_{l-m,n}(r) - \frac{\delta_{l,0}}{N_c} I_{l-m,n}^{(2)} \Phi(r) \right) (|\Phi(r)|^2 + \tilde{n}(r)) \xi_{l-m,n'}(r), \]

(C.65)

and

\[ I_{ln}^{(1)} = I_{ln}^{(2)} = \int_0^\infty dr \xi_{ln}(r) \Phi(r). \]

(C.66)

Defining the vectors \( a, c_{q,l} \) and \( d_{q,l} \) corresponding to the coefficients \( a_n, c_{q,l,n} \) and \( d_{q,l,n} \), and the matrices \( A, B, L_{q,l}^{(u)}, M_{q,l}^{(u)}, L_{q,l}^{(v)} \) and \( M_{q,l}^{(v)} \) corresponding to the matrix elements \( A_{n,n'}, B_{n,n'}, L_{q,l,n,n'}^{(u)}, M_{q,l,n,n'}^{(u)}, L_{q,l,n,n'}^{(v)} \) and \( M_{q,l,n,n'}^{(v)} \), we obtain the matrix eigenvalue equation for the coefficients for the condensate wavefunction (GGPE)

\[ \mu a = Aa \]

(C.67)

and for the quasi-particle amplitudes (BdGEs)

\[ \epsilon_{q,l} \begin{bmatrix} c_{q,l} \\ d_{q,l} \end{bmatrix} = \begin{bmatrix} L_{q,l}^{(u)} & M_{q,l}^{(u)} \\ -M_{q,l}^{(v)} & -L_{q,l}^{(v)} \end{bmatrix} \begin{bmatrix} c_{q,l} \\ d_{q,l} \end{bmatrix}. \]

(C.68)

We note that the radial Laguerre basis functions \( \xi_{ln}(r) \) given by equation (C.27) may be written as a polynomial of order \( n + l \) in \( r^2 \) times a weighting factor \( \exp(-r^2/2), \)
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thus all matrix elements are integrals of orthogonal polynomials of order $4N + 2M - 4$ in $r^2$ (since $dr^2 = 2r dr$), where we have imposed the computational mode cut-off of $n = 0, \ldots, N-1$ and $l = 0, \pm 1, \ldots, \pm M$. This facilitates the use of Gaussian quadrature for the integration (see section 5.5 in chapter 5 on numerical methods), allowing accurate computation for a minimal number of position points, greatly enhancing the efficiency and accuracy of the numerical algorithms used here.

C.2.3 Solutions for 2D BEC in Axially-symmetric trap - General Case

We consider the numerical solution for the dimensionless time-independent HFB equations (5.36) and (5.37) in the 2D case (pancake BEC) in the case where no assumptions are made concerning the axial symmetry of the solutions, in the case of no vortices, and in the case of off-axis vortices.

No Vortices

We expand the condensate wavefunction $\Phi(r, \theta)$ and quasiparticle amplitudes $u_q(r, \theta), v_q(r, \theta)$ in the Laguerre basis $\{ \xi_{ln}(r, \theta), l = 0, \pm 1, \ldots, n = 0, 1, \ldots \}$ where the $\xi_{ln}(r, \theta)$ are given by (C.26) and (C.27)

$$\xi_{ln}(r, \theta) = \frac{e^{il\theta}}{\sqrt{2\pi}} \left( \frac{2n!}{(n + |l|)!} \right)^{1/2} e^{-r^2/2} L_n^{|l|}(r^2) \equiv \xi_{ln}(r) \frac{e^{il\theta}}{\sqrt{2\pi}}.$$

$$\Phi(r, \theta) = \sum_{ln} a_{0,ln} \xi_{ln}(r, \theta) \quad (C.69)$$

$$u_q(r, \theta) = \sum_{ln} c_{q,ln} \xi_{ln}(r, \theta) \quad (C.70)$$

and

$$v_q(r, \theta) = \sum_{ln} d_{q,ln} \xi_{ln}(r, \theta). \quad (C.71)$$

Substituting (C.69) into the GGPE (5.36), and (C.70),(C.71) into the orthogonal BdGEs (5.37), we find that

$$\mu a_{ln} = \sum_{l'n'} (A_{ln,l'n'} + B_{ln,l'n'}) a_{l'n'} \quad (C.72)$$

and

$$\epsilon_q \begin{bmatrix} c_{q,ln} \\ d_{q,ln} \end{bmatrix} = \sum_{l'n'} \begin{bmatrix} L_{q,ln,l'n'}^{(u)} & M_{q,ln,l'n'}^{(u)} \\ -M_{q,ln,l'n'}^{(v)} & -L_{q,ln,l'n'}^{(v)} \end{bmatrix} \begin{bmatrix} c_{q,l'n'} \\ d_{q,l'n'} \end{bmatrix} \quad (C.73)$$
where we have defined

\[
A_{ln,l'n'} \equiv \left( \mu_{ln}^{(SP)} - l\Omega \right) \delta_{l,l'} \delta_{n,n'} + C_2D \int_0^\infty r dr d\theta \xi_{ln}(r,\theta) \left( |\Phi(r,\theta)|^2 + 2\tilde{n}(r,\theta) \right) \xi_{l'n'}(r,\theta) - P_{ln,l'n'},
\]

\[
P_{ln,l'n'} \equiv \int_0^\infty \int_0^{2\pi} \int_0^\infty r dr d\theta \left[ \tilde{n}(r',\theta',r,\theta) \left( \mu_{l'n'}^{(SP)} - l\Omega - \mu + 2C_2D \left( |\Phi(r',\theta')|^2 + \tilde{n}(r',\theta') \right) \right] \xi_{l'n'}(r',\theta')/N_c;
\]

\[
B_{ln,l'n'} \equiv C_2D \int_0^\infty r dr d\theta \xi_{ln}(r,\theta) \tilde{n}(r,\theta) \xi_{l'n'}(r,\theta),
\]

\[
L^{(u)}_{q,ln,l'n'} \equiv \left( \mu_{ln}^{(SP)} - l\Omega - \mu \right) \left( \delta_{l,l'} \delta_{n,n'} - \frac{1}{N_c} I_{ln}^{(1)} \Phi(r,\theta) \right) + I_{q,ln,l'n'},
\]

\[
L^{(v)}_{q,ln,l'n'} \equiv \left( \mu_{ln}^{(SP)} + l\Omega - \mu \right) \left( \delta_{l,l'} \delta_{n,n'} - \frac{1}{N_c} I_{ln}^{(2)} \Phi(r,\theta) \right) + I_{q,ln,l'n'},
\]

\[
M_{q,ln,l'n'}^{(u)} \equiv C_2D \int_0^\infty r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(1)} \Phi(r,\theta) \right) \left( |\Phi(r,\theta)|^2 + \tilde{n}(r,\theta) \right) \xi_{l'n'}(r,\theta),
\]

\[
M_{q,ln,l'n'}^{(v)} \equiv C_2D \int_0^\infty r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(2)} \Phi(r,\theta) \right) \left( |\Phi(r,\theta)|^2 + \tilde{n}(r,\theta) \right) \xi_{l'n'}(r,\theta),
\]

where

\[
I_{q,ln,l'n'}^{(u)} \equiv 2C_2D \int_0^\infty r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(1)} \Phi(r,\theta) \right) \left( |\Phi(r,\theta)|^2 + \tilde{n}(r,\theta) \right) \xi_{l'n'}(r,\theta),
\]

\[
I_{q,ln,l'n'}^{(v)} \equiv 2C_2D \int_0^\infty r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(2)} \Phi(r,\theta) \right) \left( |\Phi(r,\theta)|^2 + \tilde{n}(r,\theta) \right) \xi_{l'n'}(r,\theta),
\]

\[
I_{ln}^{(1)} \equiv \int_0^\infty r dr d\theta \xi_{ln}^*(r,\theta) \Phi(r,\theta)
\]

\[
I_{ln}^{(2)} \equiv \int_0^\infty r dr d\theta \xi_{ln}^*(r,\theta) \Phi(r,\theta).
\]

Defining the vectors \( \mathbf{a}, \mathbf{c}_q \) and \( \mathbf{d}_q \) corresponding to the coefficients \( a_{ln}, c_{q,ln} \) and \( d_{q,ln} \), and the matrices \( \mathbf{A}, \mathbf{B}, \mathbf{L}_q^{(u)}, \mathbf{M}_q^{(u)}, \mathbf{L}_q^{(v)} \) and \( \mathbf{M}_q^{(v)} \) corresponding to the matrix elements \( A_{ln,l'n'} \),
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\[ B_{ln',nn'}, L_{q,l,n',n}, M_{q,l,n',n}^{(u)} , L_{q,l,n',n}^{(v)} \text{ and } M_{q,l,n',n}^{(v)} \], we obtain the vector eigenvalue equation for the coefficients for the condensate wavefunction (GGPE)

\[ \mu \mathbf{a} = (\mathbf{A} + \mathbf{B}) \mathbf{a} \quad (C.85) \]

and for the quasiparticle amplitudes (BdGEs)

\[ \epsilon_q \begin{bmatrix} \mathbf{c}_q \\ \mathbf{d}_q \end{bmatrix} = \begin{bmatrix} L_q^{(u)} & M_q^{(u)} \\ -M_q^{(v)} & -L_q^{(v)} \end{bmatrix} \begin{bmatrix} \mathbf{c}_q \\ \mathbf{d}_q \end{bmatrix}. \quad (C.86) \]

Off-axis Vortices

We find stationary solutions for a single off-axis vortex by solving the 2D HFB equations (5.36) and (5.37) and the equation for the precessional frequency (4.65) self-consistently, with \( C(r, \theta) \) given by (4.125). We can write the condensate wave function \( \Phi(r, \theta) \) in terms of the modified single-particle basis \( \{ \chi_{ln}^{(1)}(r, \theta), (l, n) \in S^{(1)} \} \) for a single vortex where we have defined (5.63)

\[ S^{(1)} \equiv \{ l, n \mid (l, n) \in S - \{(1, 0)\} \} \quad (C.87) \]

with the definition \( S \equiv \{ l, n \mid n = 0, \ldots, l = 0, \pm 1, \ldots \} \) as (5.64)

\[ \Phi(r, \theta) = \sum_{l,n \in S^{(1)}} a_{ln} \chi_{ln}^{(1)}(r, \theta) \quad (C.88) \]

where (5.65)

\[ \chi_{ln}^{(1)}(r, \theta) \equiv \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_{N_v}, \theta_{N_v})}{\xi_{10}(r_{N_v}, \theta_{N_v})} \xi_{10}(r, \theta). \quad (C.89) \]

For multiple off-axis vortices we write the condensate wave function \( \Phi(r, \theta) \) in terms of the modified single-particle basis \( \{ \chi_{ln}^{(N_v)}(r, \theta), (l, n) \in S^{(N_v)} \} \) for \( N_v \) off-axis vortices situated at positions \( (r, \theta) \in \{(r_i, \theta_i) \mid i = 1, \ldots N_v\} \) as (5.69)

\[ \Phi(r, \theta) = \sum_{l,n \in S^{(N_v)}} a_{ln} \chi_{ln}^{(N_v)}(r, \theta) \quad (C.90) \]

where we have defined (5.67)

\[ S^{(N_v)} \equiv \{ l, n \mid (l, n) \in S - \{(1, 0), \ldots, (N_v, 0)\} \}; \quad (C.91) \]

and where the modified basis functions are given by (5.70)

\[ \chi_{ln}^{(N_v)}(r, \theta) \equiv \chi_{ln}^{(N_v-1)}(r, \theta) - \frac{\chi_{ln}^{(N_v-1)}(r_{N_v}, \theta_{N_v})}{\chi_{N_{v,0}}^{(N_v-1)}(r_{N_v}, \theta_{N_v})} \chi_{N_{v,0}}^{(N_v-1)}(r, \theta). \quad (C.92) \]
As before, we expand the quasiparticle amplitudes \( u_q(r, \theta) \), \( v_q(r, \theta) \) in the Laguerre basis \( \{ \xi_{ln}(r, \theta), l = 0, \pm 1, \ldots, n = 0, 1, \ldots \} \) (see (C.70),(C.71))

\[
    u_q(r, \theta) = \sum_{l,n} c_{q,ln} \xi_{ln}(r, \theta) \tag{C.93}
\]

and

\[
    v_q(r, \theta) = \sum_{l,n} d_{q,ln} \xi_{ln}(r, \theta) \tag{C.94}
\]

Substituting (C.90) into the GGPE (5.36), and (C.93),(C.94) into the orthogonal BdGEs (5.37), we find that

\[
    \mu a_{ln} = \sum_{l',n' \in S^{(1)}} (A_{ln,l'n'} + B_{ln,l'n'}) a_{l'n'} \tag{C.95}
\]

and

\[
    \epsilon_q \begin{bmatrix} c_{q,ln} \\ d_{q,ln} \end{bmatrix} = \sum_{l',n'} \begin{bmatrix} L_{q,ln,l'n'}^{(u)} & M_{q,ln,l'n'}^{(u)} \\ -M_{q,ln,l'n'}^{(v)} & -L_{q,ln,l'n'}^{(v)} \end{bmatrix} \begin{bmatrix} c_{q,l'n'} \\ d_{q,l'n'} \end{bmatrix} \tag{C.96}
\]

where we have defined

\[
    A_{ln,l'n'} \equiv \left( \mu^{(SP)}_{ln} - l \Omega \right) \delta_{l',l} \delta_{n,n'} + C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r, \theta) \left( \left| \Phi(r, \theta) \right|^2 + 2 \tilde{n}(r, \theta) \right) \chi_{l'n'}^{(N_c)}(r, \theta) - P_{ln,l'n'}, \tag{C.97}
\]

\[
    P_{ln,l'n'} \equiv \int_0^\infty \int_0^{2\pi} \int_0^\infty \int_0^{2\pi} r dr d\theta r'd\theta' d\xi_{ln}^*(r, \theta) \left[ \tilde{n}(r', \theta', r, \theta) \left( \mu^{(SP)}_{ln'} - l \Omega - \mu + 2C_{2D} \left| \Phi(r', \theta') \right|^2 + \tilde{n}(r', \theta') \right) + C_{2D} \tilde{m}(r', \theta', r, \theta) \left( \Phi^*(r', \theta') + \tilde{m}^*(r', \theta') \right) \right] \chi_{l'n'}^{(N_c)}(r', \theta') / N_c, \tag{C.98}
\]

\[
    B_{ln,l'n'} \equiv C_{2D} \int_0^\infty \int_0^{2\pi} \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r, \theta) \tilde{m}(r, \theta) \chi_{l'n'}^{(N_c)}(r, \theta), \tag{C.99}
\]

\[
    L_{q,ln,l'n'}^{(u)} \equiv \left( \mu^{(SP)}_{ln} - l \Omega - \mu \right) \left( \delta_{l',l} \delta_{n,n'} - \frac{1}{N_c} I_{ln}^{(1)} I_{l'n'}^{(1)} \right) + I_{q,ln,l'n'}^{(u)}, \tag{C.100}
\]

\[
    L_{q,ln,l'n'}^{(v)} \equiv \left( \mu^{(SP)}_{ln} + l \Omega - \mu \right) \left( \delta_{l',l} \delta_{n,n'} - \frac{1}{N_c} I_{ln}^{(2)} I_{l'n'}^{(2)} \right) + I_{q,ln,l'n'}^{(v)}, \tag{C.101}
\]

\[
    M_{q,ln,l'n'}^{(u)} \equiv C_{2D} \int_0^\infty \int_0^{2\pi} \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^*(r, \theta) - \frac{1}{N_c} I_{ln}^{(1)} \Phi(r, \theta) \right) \left( \Phi^2(r, \theta) + \tilde{m}(r, \theta) \right) \xi_{l'n'}(r, \theta), \tag{C.102}
\]

\[
    M_{q,ln,l'n'}^{(v)} \equiv C_{2D} \int_0^\infty \int_0^{2\pi} \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^*(r, \theta) - \frac{1}{N_c} I_{ln}^{(2)} \Phi(r, \theta) \right) \left( \Phi^2(r, \theta) + \tilde{m}^*(r, \theta) \right) \xi_{l'n'}(r, \theta), \tag{C.103}
\]
where

\[
I_{q,l,n,l' n'}^{(u)} \equiv 2C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^* (r, \theta) - \frac{1}{N_c} I_{ln}^{(1)} \Phi^* (r, \theta) \right) \left( |\Phi (r, \theta)|^2 + \tilde{n} (r, \theta) \right) \xi_{l' n'} (r, \theta),
\]

(C.104)

\[
I_{q,l,n,l' n'}^{(v)} \equiv 2C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^* (r, \theta) - \frac{1}{N_c} I_{ln}^{(2)} \Phi (r, \theta) \right) \left( |\Phi (r, \theta)|^2 + \tilde{n} (r, \theta) \right) \xi_{l' n'} (r, \theta),
\]

(C.105)

\[
I_{ln}^{(1)} \equiv \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^* (r, \theta) \Phi (r, \theta),
\]

(C.106)

and

\[
I_{ln}^{(2)} \equiv \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^* (r, \theta) \Phi^* (r, \theta).
\]

(C.107)

Defining the vectors \(a, c_{q,l} \) and \(d_{q,l} \) corresponding to the coefficients \(a_{ln}, c_{q,n,l} \) and \(d_{q,n,l} \), and the matrices \(A, B, L_{q}^{(u)}, M_{q}^{(u)}, L_{q}^{(v)} \) and \(M_{q}^{(v)} \) corresponding to the matrix elements \(A_{ln,l' n'}, B_{ln,l' n'}, L_{q,l,n,l',n'}^{(u)}, M_{q,l,n,l',n'}^{(u)}, L_{q,l,n,l',n'}^{(v)} \) and \(M_{q,l,n,l',n'}^{(v)} \), we obtain the vector eigenvalue equation for the coefficients for the condensate wavefunction (GGPE)

\[
\mu a = (A + B)a
\]

(C.108)

and for the quasiparticle amplitudes (BdGEs)

\[
\varepsilon \begin{bmatrix} c_q \\ d_q \end{bmatrix} = \begin{bmatrix} L_{q}^{(u)} & M_{q}^{(u)} \\ -M_{q}^{(v)} & -L_{q}^{(v)} \end{bmatrix} \begin{bmatrix} c_q \\ d_q \end{bmatrix}.
\]

(C.109)

C.2.4 Numerical Calculation of the Precessional Frequency \(\Omega\) for the Off-Axis Case

We use equation (4.65)

\[
\Omega = \frac{\int_0^{2\pi} \int_0^\infty A (r, \theta) B (r, \theta) r dr d\theta}{\int_0^{2\pi} \int_0^\infty (A (r, \theta))^2 r dr d\theta}
\]

(C.110)

to calculate the precessional frequency \(\Omega\) in the case of single and multiple off-axis vortices. Here we have defined (4.62)

\[
A (r, \theta) \equiv \left( R \frac{\partial R}{\partial \theta} + I \frac{\partial I}{\partial \theta} \right)
\]

(C.111)
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and (4.63)

\[ B(r, \theta) \equiv r^2 \left( R \frac{\partial^2 I}{\partial r^2} - i \frac{\partial^2 R}{\partial r^2} \right) + r \left( R \frac{\partial I}{\partial r} - I \frac{\partial R}{\partial r} \right) + \left( R \frac{\partial^2 I}{\partial \theta^2} - i \frac{\partial^2 R}{\partial \theta^2} \right) + \frac{i r^2}{2 \hbar} C(r, \theta) \]  

(C.112)

where \( C(r, \theta) \) is given by (4.125) and \( G(r, \theta) \) by (4.126). In the dimensionless units used here, \( C(r, \theta) \) and \( G(r, \theta) \) are given by

\[ C(r, \theta) \equiv C_{2D} \left( \tilde{m}(r, \theta) \Phi^2(r, \theta) - \tilde{m}^*(r, \theta) \Phi^2(r, \theta) \right) + G^*(r, \theta) - G(r, \theta) \]  

\[ G(r, \theta) \equiv \Phi^*(r, \theta) \int_0^{2\pi} \int_0^{\infty} rdr'd\theta' \tilde{P}(r', \theta', r, \theta) \phi(r', \theta') \]  

(C.113)

with \( \tilde{P}(r', \theta', r, \theta) \) given by (4.127). Here \( R(r, t) = \text{Re} \{ R(r, t) \} \) and \( I(r, t) = \text{Im} \{ I(r, t) \} \) represent respectively the real and imaginary parts of the condensate wavefunction

\[ R(r, t) = R(r, t) + iI(r, t). \]  

(C.114)

This requires numerical computation of the derivatives

\[ r \frac{\partial}{\partial r} \Phi(r, \theta) = \sum_{l,n \in \mathcal{S}(N_v)} a_{ln} r \frac{\partial}{\partial r} \lambda_{ln}^{(N_v)}(r, \theta), \]  

(C.115)

\[ r^2 \frac{\partial^2}{\partial r^2} \Phi(r, \theta) = \sum_{l,n \in \mathcal{S}(N_v)} a_{ln} r^2 \frac{\partial^2}{\partial r^2} \lambda_{ln}^{(N_v)}(r, \theta), \]  

(C.116)

\[ \frac{\partial}{\partial \theta} \Phi(r, \theta) = \sum_{l,n \in \mathcal{S}(N_v)} a_{ln} \frac{\partial}{\partial \theta} \lambda_{ln}^{(N_v)}(r, \theta), \]  

(C.117)

and

\[ \frac{\partial^2}{\partial \theta^2} \Phi(r, \theta) = \sum_{l,n \in \mathcal{S}(N_v)} a_{ln} \frac{\partial^2}{\partial \theta^2} \lambda_{ln}^{(N_v)}(r, \theta). \]  

(C.118)

The computation of the derivatives of the modified basis functions are evaluated analytically using the recurrence relations of the Laguerre basis functions, and the iterative relations (C.89) and (C.92) for the modified basis functions for single and multiple vortices.

Using the recurrence relation [103, 104]

\[ r \frac{dL_n^k(r)}{dr} = n L_n^k(r) - (n + k) R_{n-1}^k(r) \]  

(C.119)

for the generalised associated Laguerre polynomial \( L_n^k(r) \), and the expression (C.27) for the Laguerre basis function \( \xi_{ln}(r) = N_n^{|l|} e^{-r^2/2} r^{|l|} L_n^{|l|}(r^2) \), we find that

\[ r \frac{d\xi_{ln}(r)}{dr} = (2n + |l| - r^2) \xi_{ln}(r) - 2 \sqrt{n(n + |l|)} \xi_{l,n-1}(r) \]  

(C.120)
and

\[ r^2 \frac{d^2 \xi_{ln}(r)}{dr^2} = (2n + |l| - 1 - r^2) r \frac{d\xi_{ln}(r)}{dr} - 2r^2 \xi_{ln}(r) - 2\sqrt{n} (n + |l|) r \frac{d\xi_{l,n-1}(r)}{dr}. \]  \tag{C.121}

Now by (C.26) we can write

\[ \xi_{ln}(r, \theta) = \xi_{ln}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} \]

therefore

\[ \frac{\partial \xi_{ln}(r, \theta)}{\partial \theta} = il \xi_{ln}(r, \theta) \]  \tag{C.122}

and

\[ \frac{\partial^2 \xi_{ln}(r, \theta)}{\partial \theta^2} = -l^2 \xi_{ln}(r, \theta) \]  \tag{C.123}

Then for the case of a single off-axis vortex,

\[ r \frac{\partial}{\partial r} \chi_{ln}^{(1)}(r, \theta) \equiv r \frac{\partial}{\partial r} \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_{N_v}, \theta_{N_v})}{\xi_{10}(r_{N_v}, \theta_{N_v})} r \frac{\partial}{\partial r} \xi_{10}(r, \theta), \]  \tag{C.124}

\[ r^2 \frac{\partial^2}{\partial r^2} \chi_{ln}^{(1)}(r, \theta) \equiv r^2 \frac{\partial^2}{\partial r^2} \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_{N_v}, \theta_{N_v})}{\xi_{10}(r_{N_v}, \theta_{N_v})} r^2 \frac{\partial^2}{\partial r^2} \xi_{10}(r, \theta), \]  \tag{C.125}

\[ \frac{\partial}{\partial \theta} \chi_{ln}^{(1)}(r, \theta) \equiv \frac{\partial}{\partial \theta} \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_{N_v}, \theta_{N_v})}{\xi_{10}(r_{N_v}, \theta_{N_v})} \frac{\partial}{\partial \theta} \xi_{10}(r, \theta), \]  \tag{C.126}

and

\[ \frac{\partial^2}{\partial \theta^2} \chi_{ln}^{(1)}(r, \theta) \equiv \frac{\partial^2}{\partial \theta^2} \xi_{ln}(r, \theta) - \frac{\xi_{ln}(r_{N_v}, \theta_{N_v})}{\xi_{10}(r_{N_v}, \theta_{N_v})} \frac{\partial^2}{\partial \theta^2} \xi_{10}(r, \theta). \]  \tag{C.127}

In the case of \( N_v \) vortices, one finds that

\[ r \frac{\partial}{\partial r} \chi_{ln}^{(N_v)}(r, \theta) \equiv r \frac{\partial}{\partial r} \chi_{ln}^{(N_v-1)}(r, \theta) - \frac{\chi_{ln}^{(N_v-1)}(r_{N_v}, \theta_{N_v})}{\chi_{N_v,0}^{(N_v-1)}(r_{N_v}, \theta_{N_v})} r \frac{\partial}{\partial r} \chi_{N_v,0}^{(N_v-1)}(r, \theta), \]  \tag{C.128}

\[ r^2 \frac{\partial^2}{\partial r^2} \chi_{ln}^{(N_v)}(r, \theta) \equiv r^2 \frac{\partial^2}{\partial r^2} \chi_{ln}^{(N_v-1)}(r, \theta) - \frac{\chi_{ln}^{(N_v-1)}(r_{N_v}, \theta_{N_v})}{\chi_{N_v,0}^{(N_v-1)}(r_{N_v}, \theta_{N_v})} r^2 \frac{\partial^2}{\partial r^2} \chi_{N_v,0}^{(N_v-1)}(r, \theta), \]  \tag{C.129}

\[ \frac{\partial}{\partial \theta} \chi_{ln}^{(N_v)}(r, \theta) \equiv \frac{\partial}{\partial \theta} \chi_{ln}^{(N_v-1)}(r, \theta) - \frac{\chi_{ln}^{(N_v-1)}(r_{N_v}, \theta_{N_v})}{\chi_{N_v,0}^{(N_v-1)}(r_{N_v}, \theta_{N_v})} \frac{\partial}{\partial \theta} \chi_{N_v,0}^{(N_v-1)}(r, \theta), \]  \tag{C.130}

and

\[ \frac{\partial^2}{\partial \theta^2} \chi_{ln}^{(N_v)}(r, \theta) \equiv \frac{\partial^2}{\partial \theta^2} \chi_{ln}^{(N_v-1)}(r, \theta) - \frac{\chi_{ln}^{(N_v-1)}(r_{N_v}, \theta_{N_v})}{\chi_{N_v,0}^{(N_v-1)}(r_{N_v}, \theta_{N_v})} \frac{\partial^2}{\partial \theta^2} \chi_{N_v,0}^{(N_v-1)}(r, \theta) \]  \tag{C.131}

and one calculates these derivatives iteratively.
Appendix C. Solution of the Time-independent and Time-dependent HFB Equations

C.3 Time-dependent HFB Equations

C.3.1 Solution using RK4IP

See sections 5.4.1 and 5.4.2 in chapter 5 on numerical methods.

C.3.2 General Method of Solution using Single Particle Basis Functions

We expand the condensate wave-function \( \Phi(\vec{r}, t) \) and the quasi-particle amplitudes \( u_q(\vec{r}, t) \) and \( v_q(\vec{r}, t) \) in terms of the single-particle basis functions \( \xi_k(\vec{r}) = \xi_{\nu}(r, \theta) \zeta_k(z) \). These single-particle basis functions are solutions of the (single-particle) time-independent Schrödinger equation with respective energy eigenvalues \( \mu^{(SP)}_k \), viz.

\[
\mu^{(SP)}_k \xi_k(\vec{r}) = \hat{h}(\vec{r})\xi_k(\vec{r}).
\]  

(C.132)

Thus we may write the condensate wave function \( \Phi(\vec{r}) \) as

\[
\Phi(\vec{r}, t) = \sum_k a_k(t) \xi_k(\vec{r})
\]

(C.133)

and the quasiparticle amplitudes \( u_q(\vec{r}) \) and \( v_q(\vec{r}) \) as

\[
u_q(\vec{r}, t) = \sum_k c_q(t) \xi_k(\vec{r})
\]  

(C.134)

and

\[
v_q(\vec{r}, t) = \sum_k d_q(t) \xi_k(\vec{r})
\]  

(C.135)

respectively. We substitute (C.133) into the dimensionless modified time-dependent GGPE in the interaction picture (5.92)

\[
i \frac{\partial}{\partial t} \Phi(\vec{r}, t) = \left( \hat{h} - \mu + C_{3D} (|\Phi|^2 + 2\tilde{n}) \right) \Phi(\vec{r}, t) + C_{3D} g \tilde{n} \Phi^*(\vec{r}, t) - \int d\vec{r}' \hat{P}(r', \vec{r}, t) \phi(\vec{r}', t)
\]

(C.136)

where we have neglected \( \Delta \mu \), which we showed to be negligible in Chapter 4. Thus we obtain a matrix equation for the coefficients \( a_k(t) \) of the condensate wave-function \( \Phi(\vec{r}, t) \)

\[
i \frac{da_k(t)}{dt} = \sum_{n'} (A_{k,k'}(t)a_{k'}(t) + B_{k,k'}(t)a_{k'}^*(t))
\]

(C.137)
written in terms of the matrix elements

\[ A_{k,k'}(t) \equiv \left( \mu_{k,\Omega}^{(SP)} - m\Omega \right) \delta_{k,k'} + C_{3D} \int d\mathbf{r} \xi_k^* (\mathbf{r}) \left( |\Phi (\mathbf{r}, t)|^2 + 2\tilde{n}(\mathbf{r}, t) \right) \xi_{k'} (\mathbf{r}) - P_{k,k'}(t) \]  

(C.138)

and

\[ B_{k,k'}(t) \equiv C_{3D} \int d\mathbf{r} \xi_k^* (\mathbf{r}) \tilde{m}(\mathbf{r}, t) \xi_{k'} (\mathbf{r}) \]  

(C.139)

with

\[ P_{k,k'}(t) = \int d\mathbf{r} d\mathbf{r}' \xi_k^* (\mathbf{r}) \left[ \tilde{n}(\mathbf{r}', \mathbf{r}, t) \left( \mu_{k',\Omega}^{(SP)} + 2C_{3D} (|\Phi (\mathbf{r}', t)|^2 + \tilde{n}(\mathbf{r}', t)) \right) + C_{3D} \tilde{m}(\mathbf{r}', \mathbf{r}, t) \left( \Phi^2 (\mathbf{r}', t) + \tilde{m}^*(\mathbf{r}', t) \right) \right] \xi_{k'} (\mathbf{r}') / N_c(t). \]  

(C.140)

Similarly we substitute (C.134) and (C.135) into the dimensionless orthogonal BdGEs in the interaction picture (5.93)

\[ i \frac{\partial}{\partial t} \begin{bmatrix} u_q (\mathbf{r}, t) \\ v_q (\mathbf{r}, t) \end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix} \hat{L} (\mathbf{r}, \mathbf{r}', t, -\epsilon_q) & \mathcal{M} (\mathbf{r}, \mathbf{r}', t) \\ -\mathcal{M}^* (\mathbf{r}, \mathbf{r}', t) & -\hat{L}^* (\mathbf{r}, \mathbf{r}', t, \epsilon_q) \end{bmatrix} \begin{bmatrix} u_q (\mathbf{r}', t) \\ v_q (\mathbf{r}', t) \end{bmatrix} \]  

(C.141)

where

\[ \hat{L} (\mathbf{r}, \mathbf{r}', t, \epsilon_q) \equiv \hat{L} (\mathbf{r}, \mathbf{r}', t) + \epsilon_q \delta (\mathbf{r} - \mathbf{r}') \]  

(C.142)

where, as before

\[ \hat{L} (\mathbf{r}, \mathbf{r}', t) \equiv Q (\mathbf{r}, \mathbf{r}', t) \hat{L} (\mathbf{r}', t) \]  

\[ \mathcal{M} (\mathbf{r}, \mathbf{r}', t) \equiv Q (\mathbf{r}, \mathbf{r}', t) \mathcal{M} (\mathbf{r}', t) \]  

(C.143)

with

\[ \hat{L} (\mathbf{r}, t) \equiv \hat{h} (\mathbf{r}) - \mu + 2C_{3D} (|\Phi (\mathbf{r}, t)|^2 + \tilde{n}(\mathbf{r}, t)) \]  

\[ \mathcal{M} (\mathbf{r}, t) \equiv C_{3D} (\Phi^2 (\mathbf{r}, t) + \tilde{m}(\mathbf{r}, t)) \]  

(C.144)

to obtain a matrix equation for the coefficients \( c_{qk}(t) \) and \( d_{qk}(t) \) of the quasi-particle amplitudes \( u_q (\mathbf{r}, t) \) and \( v_q (\mathbf{r}, t) \)

\[ i \frac{d}{dt} \begin{bmatrix} c_{qk}(t) \\ d_{qk}(t) \end{bmatrix} = \sum_{k'} \begin{bmatrix} L_{q,k,k'}^{(u)} (t) & M_{q,k,k'}^{(u)} (t) \\ -M_{q,k,k'}^{(v)} (t) & -L_{q,k,k'}^{(v)} (t) \end{bmatrix} \begin{bmatrix} c_{qk}(t) \\ d_{qk}(t) \end{bmatrix} \]  

(C.145)

written in terms of the respective matrix elements

\[ L_{q,k,k'}^{(u)} (t) \equiv \left( \mu_k^{(SP)} - \mu \right) \left( \delta_{k,k'} - \frac{1}{N_c(t)} I_{k}^{(1)} (t) I_{k'}^{(1)*} (t) \right) + I_{q,k,k'}^{(u)} (t), \]  

(C.146)

\[ L_{q,k,k'}^{(v)} (t) \equiv \left( \mu_k^{(SP)} - \mu \right) \left( \delta_{k,k'} - \frac{1}{N_c(t)} I_{k}^{(2)} (t) I_{k'}^{(2)*} (t) \right) + I_{q,k,k'}^{(v)} (t), \]  

(C.147)

\[ M_{q,k,k'}^{(u)} (t) \equiv C_{3D} \int d\mathbf{r} \left( \xi_k^* (\mathbf{r}) - \frac{1}{N_c(t)} I_{k}^{(1)} (t) \Phi^* (\mathbf{r}, t) \right) \left( \Phi^2 (\mathbf{r}, t) + \tilde{m}(\mathbf{r}, t) \right) \xi_{k'} (\mathbf{r}), \]  

(C.148)
and
\[ M^{(v)}_{q,k,k'}(t) \equiv C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c(t)} I^{(2)}_{k}(t) \Phi(r,t) \right) \left( \Phi^*(r,t) + \tilde{n}(r,t) \right) \xi_{k'}(r), \] (C.149)
where
\[ I^{(u)}_{q,k,k'}(t) \equiv C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c(t)} I^{(1)}_{k}(t) \Phi^*(r,t) \right) \left( |\Phi(r,t)|^2 + \tilde{n}(r,t) \right) \xi_{k'}(r), \] (C.150)
\[ I^{(v)}_{q,k,k'}(t) \equiv C_{3D} \int dr \left( \xi^*_k(r) - \frac{1}{N_c(t)} I^{(2)}_{k}(t) \Phi(r,t) \right) \left( |\Phi(r,t)|^2 + \tilde{n}(r,t) \right) \xi_{k'}(r), \] (C.151)
\[ I^{(1)}_{k}(t) \equiv \int dr \xi^*_k(r) \Phi(r,t), \] (C.152)
and
\[ I^{(2)}_{k}(t) \equiv \int dr \xi^*_k(r) \Phi^*(r,t). \] (C.153)

Defining the vectors \( \mathbf{a}, \mathbf{c}_q \) and \( \mathbf{d}_q \) corresponding to the coefficients \( a_k, c_{q,k} \) and \( d_{q,k} \), and the matrices \( \mathbf{A}, \mathbf{B}, \mathbf{L}^{(u)}_q, \mathbf{M}^{(u)}_q, \mathbf{L}^{(v)}_q \) and \( \mathbf{M}^{(v)}_q \) corresponding to the matrix elements \( A_{k,k' \prime}, B_{k,k' \prime}, I^{(u)}_{q,k,k' \prime}, I^{(v)}_{q,k,k' \prime} \) and \( M^{(v)}_{q,k,k' \prime} \), we obtain the vector equation for the evolution of the coefficients for the condensate wavefunction (GGPE)
\[ i \frac{d \mathbf{a}(t)}{dt} = \mathbf{A} \mathbf{a}(t) + \mathbf{B}^* \mathbf{a}^*(t) \] (C.154)
which we can re-write in the form
\[ \begin{bmatrix} i \frac{d}{dt} \mathbf{a}(t) \\ i \frac{d}{dt} \mathbf{a}^*(t) \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{a}(t) \\ \mathbf{a}^*(t) \end{bmatrix}, \] (C.155)
and for the quasiparticle amplitudes (BdGEs)
\[ \begin{bmatrix} i \frac{d}{dt} \mathbf{c}_q(t) \\ i \frac{d}{dt} \mathbf{d}_q(t) \end{bmatrix} = \begin{bmatrix} \mathbf{L}^{(u)}_q & \mathbf{M}^{(u)}_q \\ -\mathbf{M}^{(v)}_q & -\mathbf{L}^{(v)}_q \end{bmatrix} \begin{bmatrix} \mathbf{c}_q(t) \\ \mathbf{d}_q(t) \end{bmatrix}. \] (C.156)

Each of these equations can be re-written in the form
\[ \frac{d \chi(t)}{dt} = \mathbf{f} (\chi(t), t) \] (C.157)
where
\[ \mathbf{f} (\chi(t), t) \equiv \mathbf{F} \chi(t). \] (C.158)

We can integrate the vector equation (C.157) using the standard fourth-order Runge-Kutta algorithm, thus
\[ \mathbf{f} (\chi(t_{n+1}), t_{n+1}) = \mathbf{f} (\chi(t_n), t_n) + \left[ k_1 + 2 (k_2 + k_3) + k_4 \right] / 6 \] (C.159)
where
\[ k_1 = f(\chi(t_n), t_n) \Delta t, \]  
\[ k_2 = f\left(\frac{\chi(t_n + \Delta t)}{2} + \frac{k_1}{2}, t_n + \frac{\Delta t}{2}\right) \Delta t, \]  
\[ k_3 = f\left(\frac{\chi(t_n + \Delta t)}{2} + \frac{k_2}{2}, t_n + \frac{\Delta t}{2}\right) \Delta t, \]  
and
\[ k_4 = f(\chi(t_n + \Delta t) + k_3, t_n + \Delta t) \Delta t. \]

### C.3.3 Solution of General 2D Case using Single Particle Basis Functions

Let us consider the quasi-2D case (pancake BEC). We expand the condensate wavefunction \( \Phi(r, \theta, t) \) and quasiparticle amplitudes \( u_q(r, \theta, t) \), \( v_q(r, \theta, t) \) in the Laguerre basis \( \left\{ \xi_{ln}(r, \theta), l = 0, \pm 1, \ldots, n = 0, 1, \ldots \right\} \) (see (C.26), (C.27))

\[ \Phi(r, \theta, t) = \sum_{ln} a_{0,ln}(t) \xi_{ln}(r, \theta) \]  
\[ u_q(r, \theta, t) = \sum_{ln} c_{q,ln}(t) \xi_{ln}(r, \theta) \]  
and
\[ v_q(r, \theta, t) = \sum_{ln} d_{q,ln}(t) \xi_{ln}(r, \theta) \]  
where
\[ \xi_{ln}(r, \theta) = \xi_{ln}(r) e^{i \theta} \sqrt{\frac{2}{\pi}}. \]

Substituting (C.164) into the GGPE (5.92), and (C.165), (C.166) into the orthogonal BdGEs (5.93) in the interaction picture, we find that
\[ i \frac{da_{ln}(t)}{dt} = \sum_{l'n'} (A_{ln,l'n'} a_{l'n'}(t) + B_{ln,l'n'} a_{l'n'}^*(t)) \]
and
\[ \frac{d}{dt} \begin{bmatrix} c_{q,ln}(t) \\ d_{q,ln}(t) \end{bmatrix} = \sum_{l'n'} \begin{bmatrix} L^{(u)}_{q,ln,l'n'} & M^{(u)}_{q,ln,l'n'} \\ -M^{(v)}_{q,ln,l'n'} & -L^{(v)}_{q,ln,l'n'} \end{bmatrix} \begin{bmatrix} c_{q,l'n'}(t) \\ d_{q,l'n'}(t) \end{bmatrix} \]

where we have defined
\[ A_{ln,l'n'}(t) \equiv A'_{ln,l'n'}(t) - P_{ln,l'n'}(t), \]  
\[ B_{ln,l'n'}(t) \equiv B'_{ln,l'n'}(t) - P_{ln,l'n'}(t), \]  
\[ L^{(u)}_{q,ln,l'n'} \equiv L^{(u)}_{q,ln,l'n'} - P_{ln,l'n'} \]  
\[ M^{(u)}_{q,ln,l'n'} \equiv M^{(u)}_{q,ln,l'n'} - P_{ln,l'n'} \]  
\[ L^{(v)}_{q,ln,l'n'} \equiv L^{(v)}_{q,ln,l'n'} - P_{ln,l'n'} \]  
\[ M^{(v)}_{q,ln,l'n'} \equiv M^{(v)}_{q,ln,l'n'} - P_{ln,l'n'} \]
Appendix C. Solution of the Time-independent and Time-dependent HFB Equations

\[ A_{ln,l'n'}(t) \equiv \left( \mu^{(SP)}_{ln} - l\Omega - \mu \right) \delta_{l,l'}\delta_{n,n'} + C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r,\theta) \left( |\Phi(r,\theta,t)|^2 + 2\tilde{n}(r,\theta,t) \right) \xi_{l'n'}(r,\theta), \]  
\[ (C.171) \]

\[ P_{ln,l'n'}(t) \equiv \int_0^\infty \int_0^{2\pi} \int_0^\infty \int_0^{2\pi} r dr d\theta' dr' d\theta' \xi_{ln}^*(r,\theta) \left[ \tilde{n}(r',\theta',r,\theta,t) \left( \mu^{(SP)}_{l'n'} - l'\Omega - \mu + 2C_{2D} \left( |\Phi(r',\theta',t)|^2 + \tilde{n}(r',\theta',t) \right) \right] + \right. \]
\[ C_{2D} \tilde{n}(r',\theta',r,\theta,t) \left( \Phi^2(r',\theta',t) + \tilde{m}^*(r',\theta',t) \right) \right] \xi_{l'n'}(r',\theta',t)/N_c(t), \]
\[ (C.172) \]

\[ B_{ln,l'n'}(t) \equiv C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r,\theta) \tilde{n}(r,\theta,t) \xi_{l'n'}^*(r,\theta), \]
\[ (C.173) \]

\[ I_{q,ln,l'n'}^{(u)}(t) \equiv \left( \mu^{(SP)}_{ln} - l\Omega - \mu - \epsilon_q \right) \left( \delta_{l,l'}\delta_{n,n'} - \frac{1}{N_c} I_{ln}^{(1)}(t) I_{l'n'}^{(1)*}(t) \right) + I_{q,ln,l'n'}^{(u)}(t), \]
\[ (C.174) \]

\[ I_{q,ln,l'n'}^{(v)}(t) \equiv \left( \mu^{(SP)}_{ln} + l\Omega - \mu + \epsilon_q \right) \left( \delta_{l,l'}\delta_{n,n'} - \frac{1}{N_c} I_{ln}^{(2)}(t) I_{l'n'}^{(2)*}(t) \right) + I_{q,ln,l'n'}^{(v)}(t), \]
\[ (C.175) \]

\[ M_{q,ln,l'n'}^{(u)}(t) \equiv C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(1)}(t) \Phi^*(r,\theta,t) \right) \left( \Phi^2(r,\theta,t) + \tilde{m}(r,\theta,t) \right) \xi_{l'n'}(r,\theta), \]
\[ (C.176) \]

and

\[ M_{q,ln,l'n'}^{(v)}(t) \equiv C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(2)}(t) \Phi(r,\theta,t) \right) \left( \Phi^2(r,\theta,t) + \tilde{m}^*(r,\theta,t) \right) \xi_{l'n'}(r,\theta), \]
\[ (C.177) \]

where

\[ I_{q,ln,l'n'}^{(u)}(t) \equiv 2C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(1)}(t) \Phi^*(r,\theta,t) \right) \left( |\Phi(r,\theta,t)|^2 + \tilde{n}(r,\theta,t) \right) \xi_{l'n'}(r,\theta), \]
\[ (C.178) \]

\[ I_{q,ln,l'n'}^{(v)}(t) \equiv 2C_{2D} \int_0^\infty \int_0^{2\pi} r dr d\theta \left( \xi_{ln}^*(r,\theta) - \frac{1}{N_c} I_{ln}^{(2)}(t) \Phi(r,\theta,t) \right) \left( |\Phi(r,\theta,t)|^2 + \tilde{n}(r,\theta,t) \right) \xi_{l'n'}(r,\theta), \]
\[ (C.179) \]

\[ I_{ln}^{(1)}(t) \equiv \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r,\theta) \Phi(r,\theta,t), \]
\[ (C.180) \]

and

\[ I_{ln}^{(2)}(t) \equiv \int_0^\infty \int_0^{2\pi} r dr d\theta \xi_{ln}^*(r,\theta) \Phi^*(r,\theta,t). \]
\[ (C.181) \]

Defining the vectors \( \mathbf{a}(t), \mathbf{c}_q(t) \) and \( \mathbf{d}_q(t) \) corresponding to the coefficients \( a_{ln}(t), c_{q,ln}(t) \) and \( d_{q,ln}(t) \), and the matrices \( \mathbf{A}, \mathbf{B}, \mathbf{L}_q^{(u)}, \mathbf{M}_q^{(u)}, \mathbf{L}_q^{(v)} \) and \( \mathbf{M}_q^{(v)} \) corresponding to the matrix
Appendix C. Solution of the Time-independent and Time-dependent HFB Equations

elements $A_{ln,l'n'}$, $B_{ln,l'n'}$, $L^{(u)}_{q,l,n,l',n'}$, $M^{(u)}_{q,l,n,l',n'}$, $L^{(v)}_{q,l,n,l',n'}$ and $M^{(v)}_{q,l,n,l',n'}$, we obtain the vector equation for the evolution of the coefficients for the condensate wavefunction (GGPE)

$$i \frac{da(t)}{dt} = Aa(t) + Ba^*(t)$$

which we can re-write in the form

$$i \frac{d}{dt} \begin{bmatrix} a(t) \\ a^*(t) \end{bmatrix} = \begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix} \begin{bmatrix} a(t) \\ a^*(t) \end{bmatrix}$$

\hspace{1cm} (C.183)

and for the quasiparticle amplitudes (BdGEs)

$$i \frac{d}{dt} \begin{bmatrix} c_q(t) \\ d_q(t) \end{bmatrix} = \begin{bmatrix} L^{(u)}_{q} & M^{(u)}_{q} \\ -M^{(v)}_{q} & -L^{(v)}_{q} \end{bmatrix} \begin{bmatrix} c_q(t) \\ d_q(t) \end{bmatrix}.$$ 

\hspace{1cm} (C.184)

Each of these equations can be re-written in the form

$$\frac{d\chi(t)}{dt} = f(\chi(t), t)$$

\hspace{1cm} (C.185)

where

$$f(\chi(t), t) \equiv F\chi(t)$$

\hspace{1cm} (C.186)

and we use the standard fourth-order Runge-Kutta algorithm as outlined in section C.3.2 above.
Appendix D

Perturbation Calculations for HFB

D.1 Calculation of Energy Shifts for Second Order Perturbation as per Morgan [23, 24]

D.1.1 Numerical Calculation

General Case

We calculate the energy shifts $\Delta \epsilon_q$ using second-order perturbation theory according to S. A. Morgan [23, 24], given by equation (2.151), thus

$$
\Delta \epsilon_q = \sum_{i,j \neq 0} \left[ -\frac{|A_{qij}|^2}{2(\epsilon_q + \epsilon_i + \epsilon_j)} (1 + n_i + n_j) + \frac{|B_{qij} + B_{qji}|}{2(\epsilon_q - \epsilon_i - \epsilon_j)} (1 + n_i + n_j) + \frac{|B_{ijq} + B_{qij}|^2}{\epsilon_q - \epsilon_i + \epsilon_j} \right] 
$$

(D.1)

where $A_{qijk} \equiv A_{ij} + A_{ikj} + A_{jik} + A_{kij} + A_{kji}$, with $A_{ij}$ and $B_{ijk}$ given by (2.147) and (2.148). In the position representation, using the contact potential approximation, $A_{ijk}$ and $B_{ijk}$ are given by (4.134)

$$
A_{ijk} = g \int d\mathbf{r} \left( \Phi^* v_i u_j u_k + \Phi u_i v_j v_k \right) 
$$

(D.2)

and (4.135)

$$
B_{ijk} = g \int d\mathbf{r} \left( \Phi^* (u_i^* u_j u_k + v_i^* v_j u_k) + \Phi \left( u_i^* u_j v_k + u_i^* v_j u_k + v_i^* v_j v_k \right) \right) 
$$

(D.3)

We find that

$$
A_{ijk} = A_{qjk} = g \int d\mathbf{r} \left( \Phi^* v_q u_j u_k + \Phi u_q v_j v_k \right),
$$
\[ A_{jkq} = A_{kjq} = g \int dr \left( \Phi^* u_q v_j u_k + \Phi v_q u_j v_k \right) \]

and

\[ A_{kaj} = A_{kjg} = g \int dr \left( \Phi^* u_q v_k u_j + \Phi v_q u_k v_j \right) \]

and therefore \( A_{qjk}^P \) can be written

\[ A_{qjk}^P = 2g \int dr \left[ (\Phi^* u_j + \Phi v_j) (v_q u_k + u_q v_k) + \Phi^* v_j u_q u_k + \Phi u_j v_q v_k \right] \quad (D.4) \]

From (D.3) we find that

\[ B_{qjk} = B_{qkj} = g \int dr \left( \Phi^* (u_q^* u_j u_k + v_q^* v_j u_k) + \Phi (u_q^* u_j v_k + u_q^* v_j u_k) \right) \]

and

\[ B_{jkq} = B_{qjk} = g \int dr \left( \Phi^* (u_q v_j^* u_k + u_q v_j^* v_k) + \Phi (v_q u_j^* u_k + u_q u_j^* v_k + v_q v_j^* v_k) \right) \]

and hence that

\[ B_{ajk} + B_{qkj} = 2g \int dr \left[ (\Phi^* u_j + \Phi v_j) (u_q^* u_k + v_q^* v_k) + \Phi^* v_j u_q^* u_k + \Phi u_j v_q^* v_k \right] \quad (D.5) \]

and

\[ B_{jkq} + B_{qjk} = 2g \int dr \left[ (\Phi^* v_j^* + \Phi u_j^*) (u_q v_k + v_q u_k) + \Phi^* u_j^* u_q u_k + \Phi v_j^* v_q v_k \right] \quad (D.6) \]

Let us define the functions

\[
\begin{align*}
 f_j^{(1)}(r) &\equiv \Phi(r) u_j(r) \\
 f_j^{(2)}(r) &\equiv \Phi^*(r) u_j(r) + \Phi(r) v_j(r) \\
 f_j^{(3)}(r) &\equiv \Phi^*(r) v_j(r) \\
 g_{qk}^{(1)}(r) &\equiv u_q(r) u_k(r) \\
 g_{qk}^{(2)}(r) &\equiv u_q(r) v_k(r) + v_q(r) u_k(r) \\
 g_{qk}^{(3)}(r) &\equiv v_q(r) v_k(r) \\
 h_{qk}^{(1)}(r) &\equiv u_q^*(r) u_k(r) \\
 h_{qk}^{(2)}(r) &\equiv u_q^*(r) v_k(r) + v_q^*(r) u_k(r) \\
 h_{qk}^{(3)}(r) &\equiv v_q^*(r) v_k(r)
\end{align*}
\]

Then

\[ A_{qjk}^P = 2g \int dr \left[ f_j^{(1)}(r) g_{qk}^{(3)}(r) + f_j^{(2)}(r) g_{qk}^{(2)}(r) + f_j^{(3)}(r) g_{qk}^{(1)}(r) \right] \quad (D.8) \]

\[ B_{ajk} + B_{qkj} = 2g \int dr \left[ f_j^{(1)}(r) h_{qk}^{(1)}(r) + f_j^{(2)}(r) h_{qk}^{(2)}(r) + f_j^{(3)}(r) h_{qk}^{(3)}(r) \right] \quad (D.9) \]

and

\[ B_{jkq} + B_{qjk} = 2g \int dr \left[ f_j^{(1)*}(r) g_{qk}^{(1)*}(r) + f_j^{(2)*}(r) g_{qk}^{(2)*}(r) + f_j^{(3)*}(r) g_{qk}^{(3)*}(r) \right] \quad (D.10) \]
Case of Axial Symmetry in 2D BEC

As before we integrate out the axial coordinate \( z \), assuming the axial confinement to be sufficiently strong that the higher axial energy modes can be ignored.

**No Vortices Present** Since no vortices are present, we can write
\[
\Phi(r, \theta) = \Phi(r) / \sqrt{2\pi} \\
u_{ln}(r, \theta) = u_{ln}(r) \exp(i l \theta) / \sqrt{2\pi} \\
v_{ln}(r, \theta) = v_{ln}(r) \exp(i l \theta) / \sqrt{2\pi}
\]

Then
\[
f_{l_j}^{(1)}(r, \theta) = f_{l_j}^{(1)}(r) \exp(i l' \theta) / \sqrt{2\pi} \\
f_{l_j}^{(2)}(r, \theta) = f_{l_j}^{(2)}(r) \exp(i l' \theta) / \sqrt{2\pi} \\
f_{l_j}^{(3)}(r, \theta) = f_{l_j}^{(3)}(r) \exp(i l' \theta) / \sqrt{2\pi} \\
g_{l_q, l''_q}(r, \theta) = g_{l_q, l''_q}(r) \exp(i (l + l'' \theta) / \sqrt{2\pi} \\
g_{l_q, l''_q}(r, \theta) = g_{l_q, l''_q}(r) \exp(i (l + l'' \theta) / \sqrt{2\pi} \\
g_{l_q, l''_q}(r, \theta) = g_{l_q, l''_q}(r) \exp(i (l + l'' \theta) / \sqrt{2\pi} \\
h_{l_q, l''_q}(r, \theta) = h_{l_q, l''_q}(r) \exp(i (l - l'' \theta) / \sqrt{2\pi} \\
h_{l_q, l''_q}(r, \theta) = h_{l_q, l''_q}(r) \exp(i (l - l'' \theta) / \sqrt{2\pi} \\
h_{l_q, l''_q}(r, \theta) = h_{l_q, l''_q}(r) \exp(i (l - l'' \theta) / \sqrt{2\pi}
\]

where
\[
f_{l_j}^{(1)}(r) = \Phi(r) u_{l_j}(r) \\
f_{l_j}^{(2)}(r) = \Phi(r) u_{l_j}(r) + \Phi(r) v_{l_j}(r) \\
f_{l_j}^{(3)}(r) = \Phi(r) v_{l_j}(r) \\
g_{l_q, l''_q}(r) = u_{l_q}(r) w_{l''_q}(r) \\
g_{l_q, l''_q}(r) = u_{l_q}(r) w_{l''_q}(r) + v_{l_q}(r) u_{l''_q}(r) \\
g_{l_q, l''_q}(r) = v_{l_q}(r) w_{l''_q}(r) \\
h_{l_q, l''_q}(r) = u_{l_q}(r) w_{l''_q}(r) \\
h_{l_q, l''_q}(r) = u_{l_q}(r) w_{l''_q}(r) + v_{l_q}(r) v_{l''_q}(r) \\
h_{l_q, l''_q}(r) = v_{l_q}(r) w_{l''_q}(r)
\]

So in the dimensionless units used here
\[
A_{l_q, l''_q}^{P} = 2 N C_{2D} R^{2} \int_{0}^{\infty} r dr \left[ f_{l_j}^{(1)}(r) g_{l_q, l''_q} + f_{l_j}^{(2)}(r) g_{l_q, l''_q} + f_{l_j}^{(3)}(r) g_{l_q, l''_q} \right] \delta_{l''_{q}, -(l' + l)} \right), \quad (D.14)
\]

\[
B_{l_q, l''_q} + B_{l_q, l''_q, l_j} = 2 N C_{2D} R^{2} \int_{0}^{\infty} r dr \left[ f_{l_j}^{(1)}(r) h_{l_q, l''_q} + f_{l_j}^{(2)}(r) h_{l_q, l''_q} + f_{l_j}^{(3)}(r) h_{l_q, l''_q} \right] \delta_{l''_{q}, l + l'}, \quad (D.15)
\]

and
\[
B_{l_q, l''_q} + B_{l_q, l''_q, l_j} = 2 N C_{2D} R^{2} \int_{0}^{\infty} r dr \left[ f_{l_j}^{(1)}(r) g_{l_q, l''_q} + f_{l_j}^{(2)}(r) g_{l_q, l''_q} + f_{l_j}^{(3)}(r) g_{l_q, l''_q} \right] \delta_{l''_{q}, l + l'}. \quad (D.16)
\]
Appendix D. Perturbation Calculations for HFB

**Single on-axis Vortex**  For a single on-axis vortex of charge \( m \), we can write

\[
\Phi(r, \theta) = \frac{\Phi(r)}{\exp(i m \theta)\sqrt{2\pi}}
\]

\[
u_{ln}(r, \theta) = \sqrt{2\pi} \exp(i (l + m) \theta)
\]

\[
v_{ln}(r, \theta) = \sqrt{2\pi} \exp(i (l - m) \theta)
\]

Then

\[
f_{ij}^{(1)}(r, \theta) = f_{ij}^{(1)}(r) \exp(i (l' + 2m) \theta)\sqrt{2\pi}
\]

\[
f_{ij}^{(2)}(r, \theta) = f_{ij}^{(2)}(r) \exp(i l' \theta)\sqrt{2\pi}
\]

\[
f_{ij}^{(3)}(r, \theta) = f_{ij}^{(3)}(r) \exp(i (l' - 2m) \theta)\sqrt{2\pi}
\]

\[
g_{iq,vk}^{(1)}(r, \theta) = g_{iq,vk}^{(1)}(r) \frac{i (l + l'' + 2m) \theta}{\sqrt{2\pi}}
\]

\[
g_{iq,vk}^{(2)}(r, \theta) = g_{iq,vk}^{(2)}(r) \frac{i (l + l'') \theta}{\sqrt{2\pi}}
\]

\[
g_{iq,vk}^{(3)}(r, \theta) = g_{iq,vk}^{(3)}(r) \frac{i (l + l'' - 2m) \theta}{\sqrt{2\pi}}
\]

\[
h_{iq,vk}^{(1)}(r, \theta) = h_{iq,vk}^{(1)}(r) \frac{i (-l + l'' + 2m) \theta}{\sqrt{2\pi}}
\]

\[
h_{iq,vk}^{(2)}(r, \theta) = h_{iq,vk}^{(2)}(r) \frac{i (-l + l'') \theta}{\sqrt{2\pi}}
\]

\[
h_{iq,vk}^{(3)}(r, \theta) = h_{iq,vk}^{(3)}(r) \frac{i (-l + l'' - 2m) \theta}{\sqrt{2\pi}}
\]

where

\[
f_{ij}^{(1)}(r) = \Phi(r) u_{ij}(r)
\]

\[
f_{ij}^{(2)}(r) = \Phi(r) u_{ij}(r) + \Phi(r) v_{ij}(r)
\]

\[
f_{ij}^{(3)}(r) = \Phi(r) v_{ij}(r)
\]

\[
g_{iq,vk}^{(1)}(r) = u_{iq}(r) u_{vk}(r)
\]

\[
g_{iq,vk}^{(2)}(r) = u_{iq}(r) v_{vk}(r) + v_{iq}(r) u_{vk}(r)
\]

\[
g_{iq,vk}^{(3)}(r) = v_{iq}(r) v_{vk}(r)
\]

\[
h_{iq,vk}^{(1)}(r) = u_{iq}(r) v_{vk}(r)
\]

\[
h_{iq,vk}^{(2)}(r) = u_{iq}(r) u_{vk}(r) + v_{iq}(r) v_{vk}(r)
\]

\[
h_{iq,vk}^{(3)}(r) = v_{iq}(r) u_{vk}(r)
\]

So in the dimensionless units used here

\[
A_{iq,jv;vk}^{\mathcal{P}} = 2NC_{2D}^R \int_0^{\infty} r dr \left[ f_{ij}^{(1)} g_{iq,vk}^{(3)} + f_{ij}^{(2)} g_{iq,vk}^{(2)} + f_{ij}^{(3)} g_{iq,vk}^{(1)} \right] \delta_{\nu',-l''-v'}
\]

\[
B_{jq,i;v;kv} + B_{jq,v;ki} = 2NC_{2D}^R \int_0^{\infty} r dr \left[ f_{ij}^{(1)} h_{iq,vk}^{(1)} + f_{ij}^{(2)} h_{iq,vk}^{(2)} + f_{ij}^{(3)} h_{iq,vk}^{(3)} \right] \delta_{\nu'-l'-v}
\]

and

\[
B_{jq,i;v;kv} + B_{jq,v;ki} = 2NC_{2D}^R \int_0^{\infty} r dr \left[ f_{ij}^{(1)} g_{iq,vk}^{(1)} + f_{ij}^{(2)} g_{iq,vk}^{(2)} + f_{ij}^{(3)} g_{iq,vk}^{(3)} \right] \delta_{\nu'+l'+v}
\]

as in the case of no vortices.
D.1.2 Equivalence of Morgan’s Generalised BdGEs [23, 24] of the form (2.156), and of the Modified Orthogonal Time-independent BdGEs (4.143)

We first note that we can rewrite equations (D.4), (D.5), and (D.6) in the forms

\[ A_{qij}^{F3} = 2g \int dr \left[ u_q(r)a_{ij}^{(1)}(r) + v_q(r)a_{ij}^{(2)}(r) \right], \]  
\[ B_{qij} + B_{qji} = 2g \int dr \left[ u_q(r)a_{ij}^{(2)}(r) + v_q(r)a_{ij}^{(1)}(r) \right] \]  
and
\[ B_{ijq} + B_{iqj} = 2g \int dr \left[ u_q(r)b_{ij}^{(1)}(r) + v_q(r)b_{ij}^{(2)}(r) \right] \]

where

\[ a_{ij}^{(1)}(r) \equiv u_j(r)f_i^{(3)}(r) + v_j(r)f_i^{(2)}(r), \]  
\[ a_{ij}^{(2)}(r) \equiv v_j(r)f_i^{(1)}(r) + u_j(r)f_i^{(2)}(r), \]  
\[ b_{ij}^{(1)}(r) \equiv u_j(r)f_i^{(1)*}(r) + v_j(r)f_i^{(2)*}(r), \]  
and
\[ b_{ij}^{(2)}(r) \equiv v_j(r)f_i^{(3)*}(r) + u_j(r)f_i^{(2)*}(r). \]

Then, defining

\[ E^{(A)}_{qij} \equiv -\frac{1 + n_i + n_j}{2(\epsilon_q + \epsilon_i + \epsilon_j)}, \]  
\[ E^{(B1)}_{qij} \equiv \frac{1 + n_i + n_j}{2(\epsilon_q - \epsilon_i - \epsilon_j)} \]  
and
\[ E^{(B2)}_{qij} \equiv \frac{n_j - n_i}{\epsilon_q - \epsilon_i - \epsilon_j} \]

we find that we can re-write equation (D.1) for \( \Delta \epsilon_q \) in the form

\[ \Delta \epsilon_q = \int dr dr' \left[ u_q^*(r) \Delta \mathcal{L}'(r, r', \epsilon_q) u_q(r') + u_q^*(r) \Delta \mathcal{M}'(r, r', \epsilon_q) v_q(r') \right. \]
\[ \left. + v_q^*(r) \Delta \mathcal{M}'(r, r', -\epsilon_q) u_q(r') + v_q^*(r) \Delta \mathcal{L}'(r, r', -\epsilon_q) v_q(r') \right] \]

with

\[ \Delta \mathcal{L}'(r, r', \epsilon_q) \equiv 4g^2 \sum_{ij} \left[ a_{ij}^{(1)*}(r)a_{ij}^{(1)*}(r')E^{(A)}_{qij} + a_{ij}^{(2)*}(r)a_{ij}^{(2)*}(r')E^{(B1)}_{qij} + b_{ij}^{(1)*}(r)b_{ij}^{(1)*}(r')E^{(B2)}_{qij} \right] \]  
(D.34)
\[ \Delta \mathcal{M}'(\mathbf{r}, \mathbf{r}', \epsilon_q) \equiv 4g^2 \sum_{ij} \left[ a_{ij}^{(1)*}(\mathbf{r}) a_{ij}^{(2)}(\mathbf{r}') E_{qij}^{(A)} + a_{ij}^{(2)}(\mathbf{r}) a_{ij}^{(1)*}(\mathbf{r}') E_{qij}^{(B1)} + b_{ij}^{(1)*}(\mathbf{r}) b_{ij}^{(2)}(\mathbf{r}') E_{qij}^{(B2)} \right], \]

which is consistent with writing the modified orthogonal time-independent BdGEs (4.107) in the form (4.143)

\[
\begin{equation}
\begin{bmatrix}
\epsilon_q u_q(\mathbf{r}) \\
v_q(\mathbf{r})
\end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix}
\hat{\mathcal{L}}^{(P)}(\mathbf{r}, \mathbf{r}', \epsilon_q) & \mathcal{M}^{(P)}(\mathbf{r}, \mathbf{r}', \epsilon_q) \\
-M^{(P)*}(\mathbf{r}, \mathbf{r}', -\epsilon_q) & -\hat{\mathcal{L}}^{(P)*}(\mathbf{r}, \mathbf{r}', -\epsilon_q)
\end{bmatrix} \begin{bmatrix}
u_q(\mathbf{r})
\end{bmatrix}
\end{equation}
\]

(D.36)

where we have defined

\[
\begin{align*}
\hat{\mathcal{L}}^{(P)}(\mathbf{r}, \mathbf{r}', \epsilon_q) & \equiv \hat{\mathcal{L}}(\mathbf{r}, \mathbf{r}') + \Delta \mathcal{L}(\mathbf{r}, \mathbf{r}', \epsilon_q) \\
\mathcal{M}^{(P)}(\mathbf{r}, \mathbf{r}', \epsilon_q) & \equiv \mathcal{M}(\mathbf{r}, \mathbf{r}') + \Delta \mathcal{M}(\mathbf{r}, \mathbf{r}', \epsilon_q)
\end{align*}
\]

(D.37)

with

\[
\begin{align*}
\Delta \mathcal{L}(\mathbf{r}, \mathbf{r}', \epsilon_q) & \equiv \int d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}'') \Delta \mathcal{L}'(\mathbf{r}'', \mathbf{r}', \epsilon_q) \\
\Delta \mathcal{M}(\mathbf{r}, \mathbf{r}', \epsilon_q) & \equiv \int d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}'') \Delta \mathcal{M}'(\mathbf{r}'', \mathbf{r}', \epsilon_q).
\end{align*}
\]

(D.38)

This ensures the orthogonality of the condensate and non-condensate since

\[
\int d\mathbf{r} \phi^*(\mathbf{r}) \int d\mathbf{r}' \Delta \mathcal{L}(\mathbf{r}, \mathbf{r}', \epsilon_q) u_q(\mathbf{r}') = \int d\mathbf{r} \phi^*(\mathbf{r}) \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}'') \Delta \mathcal{L}'(\mathbf{r}'', \mathbf{r}', \epsilon_q) u_q(\mathbf{r}')
\]

\[
= \int d\mathbf{r} \phi^*(\mathbf{r}) \int d\mathbf{r}' \Delta \mathcal{L}'(\mathbf{r}, \mathbf{r}', \epsilon_q) u_q(\mathbf{r}')
- \int d\mathbf{r} |\phi(\mathbf{r})|^2 \int d\mathbf{r}' d\mathbf{r}'' \phi^*(\mathbf{r}'') \Delta \mathcal{L}'(\mathbf{r}'', \mathbf{r}', \epsilon_q) u_q(\mathbf{r}')
\]

\[
= 0
\]

and

\[
\int d\mathbf{r} \phi^*(\mathbf{r}) \int d\mathbf{r}' \Delta \mathcal{M}(\mathbf{r}, \mathbf{r}', \epsilon_q) v_q(\mathbf{r}') = \int d\mathbf{r} \phi^*(\mathbf{r}) \int d\mathbf{r}' d\mathbf{r}'' Q(\mathbf{r}, \mathbf{r}'') \Delta \mathcal{M}'(\mathbf{r}'', \mathbf{r}', \epsilon_q) v_q(\mathbf{r}')
\]

\[
= \int d\mathbf{r} \phi^*(\mathbf{r}) \int d\mathbf{r}' \Delta \mathcal{M}'(\mathbf{r}, \mathbf{r}', \epsilon_q) v_q(\mathbf{r}')
- \int d\mathbf{r} |\phi(\mathbf{r})|^2 \int d\mathbf{r}' d\mathbf{r}'' \phi^*(\mathbf{r}'') \Delta \mathcal{M}'(\mathbf{r}'', \mathbf{r}', \epsilon_q) v_q(\mathbf{r}')
\]

\[
= 0.
\]
Appendix D. Perturbation Calculations for HFB

D.2 Perturbative Calculation of Energy Shifts due to Exclusion of $\tilde{m}$

D.2.1 The Perturbation Equations for Orthogonal HFB

The Time-independent Equations for the Condensate and Quasiparticle Amplitudes in the Orthogonal Formalism

The unperturbed orthogonal HFB equations (4.106) and (4.107) can be written in the form

$$\mu \Phi(r) = \int dr' \left[ \hat{F}(r, r') \Phi(r') + \hat{G}(r, r') \Phi^*(r') \right]$$

(D.39)

for the GGPE, and

$$\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \int dr' \begin{bmatrix} \hat{L}(r, r') & \hat{M}(r, r') \\ -\hat{M}^*(r, r') & -\hat{L}^*(r, r') \end{bmatrix} \begin{bmatrix} u_q(r') \\ v_q(r') \end{bmatrix}$$

(D.40)

for the BdGEs, where

$$\begin{align*}
\hat{F}(r, r') &\equiv \hat{F}(r) \delta(r - r') - \hat{P}(r, r') / \sqrt{N_c} \\
\hat{G}(r, r') &\equiv \hat{G}(r) \delta(r - r') \\
\hat{F}(r) &\equiv \hat{h}(r) + g (|\Phi(r)|^2 + 2\tilde{n}(r)) \\
\hat{G}(r) &\equiv g\tilde{m}(r) \\
\hat{L}(r, r') &\equiv Q(r, r') \hat{L}(r') \\
\hat{M}(r, r') &\equiv Q(r, r') \hat{M}(r') \\
\hat{L}(r) &\equiv \hat{h}(r) - \mu + 2g (|\Phi(r)|^2 + \tilde{n}(r)) \\
\hat{M}(r) &\equiv g (\Phi^2(r) + \tilde{m}(r)).
\end{align*}$$

(D.41)

Here we have neglected $\Delta \mu$ in the GGPE. We would expect $\Delta \mu$ to be insignificant compared to the energy shifts for large $N$, and therefore omit $\Delta \mu$ for simplicity. $\Delta \mu$ could be included, if required, and calculated from the number of condensate atoms $N_c$ using the Bose distribution, and solved self-consistently with the time-independent HFB equations and the equations for the energy shifts. Let us consider perturbations $\Delta \hat{F}(r, r')$, $\Delta \hat{G}(r, r')$, $\Delta \hat{L}(r, r')$, and $\Delta \hat{M}(r, r')$ to $\hat{F}(r, r')$, $\hat{G}(r, r')$, $\hat{L}(r, r')$, and $\hat{M}(r, r')$ respectively. Then we can write the perturbed orthogonal HFB equations in the form

$$\mu \Phi(r) = \int dr' \left[ \left( \hat{F}(r, r') + \Delta \hat{F}(r, r') \right) \Phi(r') + \left( \hat{G}(r, r') + \Delta \hat{G}(r, r') \right) \Phi^*(r') \right]$$

(D.42)
for the GGPE, and
\[
\epsilon_q \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} = \int dr' \begin{bmatrix} (\hat{L}(r, r') + \Delta \hat{L}(r, r')) & (\hat{M}(r, r') + \Delta \hat{M}(r, r')) \\ (\hat{M}^*(r, r') + \Delta \hat{M}^*(r, r')) & (\hat{L}^*(r, r') + \Delta \hat{L}^*(r, r')) \end{bmatrix} \begin{bmatrix} u_q(r') \\ v_q(r') \end{bmatrix}
\] (D.43)
for the BdGEs with
\[
\begin{align*}
\Delta \hat{L}(r, r') & \equiv Q(r, r') \Delta \hat{L}(r') \\
\Delta \hat{M}(r, r') & \equiv Q(r, r') \Delta \hat{M}(r').
\end{align*}
\] (D.44)

### The Perturbation Equations for the GGPE

From equation (D.39), the \( n \)th eigenvector equation for the unperturbed system is given by
\[
\mu_n(0) \phi_n(0)(r) = \int dr' \left[ \hat{F}(r, r') \phi_n(0)(r') + \hat{G}(r, r') \phi_n(0)^*(r') \right]
\] (D.45)
The corresponding equation for the time-independent perturbed system is given by
\[
\mu_n \phi_n(r) = \int dr' \left[ \left( \hat{F}(r, r') + \Delta \hat{F}(r, r') \right) \phi_n(r') + \left( \hat{G}(r, r') + \Delta \hat{G}(r, r') \right) \phi_n^*(r') \right]
\] (D.46)
where
\[
\begin{align*}
\mu_n & = \mu_n^{(0)} + \mu_n^{(1)} + \mu_n^{(2)} + \cdots \\
\phi_n(r) & = \phi_n^{(0)}(r) + \phi_n^{(1)}(r) + \phi_n^{(2)}(r) + \cdots
\end{align*}
\] (D.47)
and where \( \mu_n^{(0)}, \mu_n^{(1)}, \mu_n^{(2)}, \ldots \) and \( \phi_n^{(0)}(r), \phi_n^{(1)}(r), \phi_n^{(2)}(r), \ldots \) represent the chemical potential and the GGPE eigenvectors (normalised to unity) perturbed to zeroth order (unperturbed system), to first order, to second order, etc. Let us define the state vector
\[
\chi(r) \equiv \begin{bmatrix} \phi_n(r) \\ \phi_n^*(r) \end{bmatrix}
\] (D.48)
and the matrix operators
\[
\begin{align*}
\hat{K}(r, r') & \equiv \begin{bmatrix} \hat{F}(r, r') & \hat{G}(r, r') \\ \hat{G}^*(r, r') & \hat{F}^*(r, r') \end{bmatrix}, \\
\Delta \hat{K}(r, r') & \equiv \begin{bmatrix} \Delta \hat{F}(r, r') & \Delta \hat{G}(r, r') \\ \Delta \hat{G}^*(r, r') & \Delta \hat{F}^*(r, r') \end{bmatrix}.
\end{align*}
\] (D.49)
Then we can write
\[
\mu_n^{(0)} \chi_n^{(0)}(r) = \int dr' \hat{K}(r, r') \chi_n^{(0)}(r')
\] (D.50)
for the unperturbed system, and
\[
\mu_n \chi_n(r) = \int dr' \left[ \hat{K}(r, r') + \Delta \hat{K}(r, r') \right] \chi_n(r')
\] (D.51)
for the perturbed system.

We define a generalised inner product for the two-vectors $a_m(r), b_n(r)$ as follows

$$ (a_m(r), b_n(r))_\pm \equiv \int dr \left[ (a_m^*(r))^T S_\pm b_n(r) \right] $$  \hspace{2cm} (D.52)

where

$$ S_\pm = \begin{bmatrix} 1 & 0 \\ 0 & \pm 1 \end{bmatrix} $$  \hspace{2cm} (D.53)

We note that

$$ (\chi_m(r), \chi_n(r))_+ = 2\delta_{m,n} $$  \hspace{2cm} (D.54)

for the condensate wavefunction. We can now apply standard perturbation theory utilising this generalised inner product. We find that

$$ \mu_0^{(1)} = \frac{1}{2} \left( \chi_0^{(0)}(r), \int dr' \Delta \hat{K}(r, r') \chi_0^{(0)}(r') \right)_+ $$  \hspace{2cm} (D.55)

and

$$ \mu_0^{(2)} = \sum_{n \neq 0} \frac{\left( \chi_0^{(0)}(r), \int dr' \Delta \hat{K}(r, r') \chi_n^{(0)}(r') \right)_+ \left( \chi_n^{(0)}(r), \int dr' \Delta \hat{K}(r, r') \chi_0^{(0)}(r') \right)_+}{4 \left( \mu_0^{(0)} - \mu_n^{(0)} \right)} $$  \hspace{2cm} (D.56)

where $N_c$ is the condensate number. The first and second order shifts in the chemical potential $\mu$ are given by the ensemble averages $\Delta \mu^{(1)} = \langle \mu_0^{(1)} \rangle$ and $\Delta \mu^{(2)} = \langle \mu_0^{(2)} \rangle$. The first and second order shifts are therefore given by

$$ \Delta \mu^{(1)} = \frac{1}{2} \left\langle \left( \chi_0^{(0)}(r), \int dr' \Delta \hat{K}(r, r') \chi_0^{(0)}(r') \right)_+ \right\rangle $$  \hspace{2cm} (D.57)

and

$$ \Delta \mu^{(2)} = \sum_{n \neq 0} \frac{\left\langle \left( \chi_0^{(0)}(r), \int dr' \Delta \hat{K}(r, r') \chi_n^{(0)}(r') \right)_+ \left( \chi_n^{(0)}(r), \int dr' \Delta \hat{K}(r, r') \chi_0^{(0)}(r') \right)_+ \right\rangle}{4 \left( \mu_0^{(0)} - \mu_n^{(0)} \right)} $$  \hspace{2cm} (D.58)

The Perturbation Equations for the BdGEs

From the orthogonal BdGEs (D.40) for the unperturbed system, and (D.43) for the perturbed system, the $n$th eigenvector equation for the unperturbed system is given by

$$ e_q^{(0)} w_q^{(0)}(r) = \int dr' \hat{L}(r, r') w_q^{(0)}(r') $$  \hspace{2cm} (D.59)
and the corresponding equation for the perturbed system (D.43) is given by

\[ \epsilon_q w_q(r) = \int dr' \left\{ \left( \hat{L}(r, r') + \Delta \hat{L}(r, r') \right) \right\} w_q(r'), \tag{D.60} \]

where we have defined the state vectors

\[ w_q^{(0)}(r) = \begin{bmatrix} u_q^{(0)}(r) \\ v_q^{(0)}(r) \end{bmatrix}, \quad w_q(r) = \begin{bmatrix} u_q(r) \\ v_q(r) \end{bmatrix} \tag{D.61} \]

for the unperturbed and perturbed system, and the matrix operators

\[ \hat{L}(r, r') \equiv \begin{bmatrix} \hat{\mathcal{L}}(r, r') & \hat{\mathcal{M}}(r, r') \\ -\hat{\mathcal{M}}^*(r, r') & -\hat{\mathcal{L}}^*(r, r') \end{bmatrix}, \quad \Delta \hat{L}(r, r') \equiv \begin{bmatrix} \Delta \hat{\mathcal{L}}(r, r') & \Delta \hat{\mathcal{M}}(r, r') \\ -\Delta \hat{\mathcal{M}}^*(r, r') & -\Delta \hat{\mathcal{L}}^*(r, r') \end{bmatrix}. \tag{D.62} \]

Let us write

\[ \epsilon_q = \epsilon_q^{(0)} + \epsilon_q^{(1)} + \epsilon_q^{(2)} + \cdots \]

\[ w_q(r) = w_q^{(0)}(r) + w_q^{(1)}(r) + w_q^{(2)}(r) + \cdots \tag{D.63} \]

where \( \epsilon_q^{(0)}, \epsilon_q^{(1)}, \epsilon_q^{(2)}, \cdots \) and \( w_q^{(0)}(r), w_q^{(1)}(r), w_q^{(2)}(r), \cdots \) represent the quasiparticle excitation energies and amplitudes perturbed to zeroth order (unperturbed system), to first order, to second order, etc. We use standard perturbation theory and expand \( w_q^{(s)}(r) \) in terms of the unperturbed eigenvectors \( \left\{ w_k^{(0)}(r) \right\} \) as follows

\[ w_q^{(s)}(r) = \sum_k c_{qk}^{(s)} w_k^{(0)}(r) \tag{D.64} \]

We note that

\[ (w_p(r), w_q(r))_\perp = k\delta_{p,q} \tag{D.65} \]

where

\[ k = \begin{cases} 1 & \text{for dimensioned units} \\ 1/N_{\text{atoms}} & \text{for dimensionless units used here} \end{cases} \tag{D.66} \]

for the quasiparticle amplitudes. Utilising this generalised inner product. We find that

\[ \epsilon_q^{(1)} = \frac{1}{k} \left( w_q^{(0)}(r), \int dr' \Delta \hat{\mathcal{L}}(r, r') w_q^{(0)}(r') \right)_\perp \tag{D.67} \]

and

\[ \epsilon_q^{(2)} = \sum_{n \neq 0} \frac{\left( w_n^{(0)}(r), \int dr' \Delta \hat{\mathcal{L}}(r, r') w_q^{(0)}(r') \right)_\perp \left( w_q^{(0)}(r), \int dr' \Delta \hat{\mathcal{L}}(r, r') w_n^{(0)}(r') \right)_\perp}{k^2 \left( \epsilon_q^{(0)} - \epsilon_n^{(0)} \right)} \tag{D.68} \]

The first and second order shifts in the quasi-particle excitation energies \( \epsilon_q \) are given by the ensemble averages \( \Delta \epsilon_q^{(1)} = \langle \epsilon_q^{(1)} \rangle \) and \( \Delta \epsilon_q^{(2)} = \langle \epsilon_q^{(2)} \rangle \). The first and second order shifts are therefore given by

\[ \Delta \epsilon_q^{(1)} = \frac{1}{k} \left\langle \left( w_q^{(0)}(r), \int dr' \Delta \hat{\mathcal{L}}(r, r') w_q^{(0)}(r') \right)_\perp \right\rangle \tag{D.69} \]
Appendix D. Perturbation Calculations for HFB

\[ \Delta \mu^{(2)}_q = \sum_{n \neq 0} \frac{\left\langle \left( w_n^{(0)}(r), \int dr' \Delta \mathbf{L}(r, r') w_q^{(0)}(r') \right) - \left( w_q^{(0)}(r), \int dr' \Delta \mathbf{L}(r, r') w_n^{(0)}(r') \right) \right\rangle}{k^2 (\epsilon_q^{(0)} - \epsilon_n^{(0)})}. \]  

(D.70)

D.2.2 Calculation of shifts in Chemical Potential and Quasiparticle Energies due to Neglect of the Anomalous Density \( \tilde{m}(r) \)

We can apply first-order and second-order perturbation theory to remove the effect of the anomalous density \( \tilde{m}(r) \). This yields a Popov-type energy spectrum, thereby eliminating the energy gap problem, but does not violate conservation laws as is the case with the usual Popov approximation. This perturbation can be used to obtain a good approximate solution without incurring the computational overhead in applying Morgan’s perturbation result [23, 24] to calculate the energy shifts self-consistently with the orthogonal HFB equations. We do this by setting \( \Delta \tilde{F}(r, r') = 0, \Delta \tilde{G}(r, r') = -g\tilde{m}(r)\delta(r-r'), \Delta \tilde{L}(r, r') = 0 \) and \( \Delta \tilde{M}(r, r') = -g\tilde{m}(r)Q(r, r'), \) thus

\[
\Delta \tilde{K}(r) \equiv \begin{bmatrix} 0 & -g\tilde{m}(r)\delta(r-r') \\ -g\tilde{m}^*(r)\delta(r-r') & 0 \end{bmatrix} \quad \text{(D.71)}
\]

and

\[
\Delta \tilde{L}(r, r') \equiv \begin{bmatrix} 0 & -gQ(r, r')\tilde{m}^*(r') \\ gQ^*(r, r')\tilde{m}(r') & 0 \end{bmatrix} \quad \text{(D.72)}
\]

Then

\[
\left( \chi_0^{(0)}(r), \int dr' \Delta \tilde{K}(r, r') \chi_0^{(0)}(r') \right)_+ = g \int dr \left( \phi_0^2(r)\tilde{m}^*(r) + \phi_0^{*2}(r)\tilde{m}(r) \right),
\]

\[
\left( \chi_n^{(0)}(r), \int dr' \Delta \tilde{K}(r, r') \chi_n^{(0)}(r') \right)_+ = g \int dr \left( \phi_0(r)\phi_n(r)\tilde{m}^*(r) + \phi_0^{*}(r)\phi_n^*(r)\tilde{m}(r) \right),
\]

and

\[
\left( \chi_n^{(0)}(r), \int dr' \Delta \tilde{K}(r, r') \chi_0^{(0)}(r') \right)_+ = g \int dr \left( \phi_n(r)\phi_0(r)\tilde{m}^*(r) + \phi_n^{*}(r)\phi_0^*(r)\tilde{m}(r) \right).
\]

Therefore by equations (D.57) and (D.58)

\[
\Delta \mu^{(1)} = -\frac{g}{2} \int dr \left( \phi_0^2\tilde{m}^* + \phi_0^{*2}\tilde{m} \right) \quad \text{(D.73)}
\]
and
\[ \Delta \mu^{(2)} = g^2 \sum_{n \neq 0} \int d\mathbf{r} \left( \phi_0 \phi_n \hat{m}^* + \phi_0^* \phi_n^* \hat{m} \right) \int d\mathbf{r} \left( \phi_n \phi_0 \hat{m}^* + \phi_n^* \phi_0^* \hat{m} \right) \frac{4 \left( \mu_0^{(0)} - \mu_n^{(0)} \right)}{4 \left( \mu_0^{(0)} - \mu_n^{(0)} \right)}. \] 

Furthermore
\[ \left( \mathbf{w}_n^{(0)}(\mathbf{r}), \int d\mathbf{r}' \Delta \hat{L}(\mathbf{r}, \mathbf{r}') \mathbf{w}_q^{(0)}(\mathbf{r}') \right) = g \int d\mathbf{r} \left( u_n^{(0)*}(\mathbf{r})v_q^{(0)}(\mathbf{r})\hat{m}(\mathbf{r}) + u_q^{(0)}(\mathbf{r})v_q^{(0)*}(\mathbf{r})\hat{m}^*(\mathbf{r}) \right) , \]
\[ \left( \mathbf{w}_n^{(0)}(\mathbf{r}), \int d\mathbf{r}' \Delta \hat{L}(\mathbf{r}, \mathbf{r}') \mathbf{w}_n^{(0)}(\mathbf{r}') \right) = g \int d\mathbf{r} \left( u_n^{(0)*}(\mathbf{r})v_n^{(0)}(\mathbf{r})\hat{m}(\mathbf{r}) + v_n^{(0)*}(\mathbf{r})u_n^{(0)}(\mathbf{r})\hat{m}^*(\mathbf{r}) \right) , \]
and
\[ \left( \mathbf{w}_q^{(0)}(\mathbf{r}), \int d\mathbf{r}' \Delta \hat{L}(\mathbf{r}, \mathbf{r}') \mathbf{w}_q^{(0)}(\mathbf{r}') \right) = g \int d\mathbf{r} \left( u_q^{(0)*}(\mathbf{r})v_q^{(0)}(\mathbf{r})\hat{m}(\mathbf{r}) + v_q^{(0)*}(\mathbf{r})u_q^{(0)}(\mathbf{r})\hat{m}^*(\mathbf{r}) \right) , \]
and therefore by equations (D.69) and (D.70), the first and second order shifts in the quasi-particle excitation energies are given respectively by
\[ \Delta \epsilon_q^{(1)} = \frac{1}{k} \left\langle \left( \mathbf{w}_q^{(0)}(\mathbf{r}), \int d\mathbf{r}' \Delta \hat{L}(\mathbf{r}, \mathbf{r}') \mathbf{w}_q^{(0)}(\mathbf{r}') \right) - \right\rangle = -\frac{g}{k} \int d\mathbf{r} \left( u_q^{(0)*}v_q^{(0)}\hat{m} + u_q^{(0)}v_q^{(0)*}\hat{m}^* \right) \] 
(D.75)
and
\[ \Delta \epsilon_q^{(2)} = g^2 \sum_{n \neq 0} \int d\mathbf{r} \left( u_n^{(0)*}v_q^{(0)}\hat{m} + v_n^{(0)*}u_q^{(0)}\hat{m}^* \right) \int d\mathbf{r} \left( u_q^{(0)*}v_n^{(0)}\hat{m} + v_q^{(0)*}u_n^{(0)}\hat{m}^* \right) \frac{4 \left( \epsilon_q^{(0)} - \epsilon_n^{(0)} \right)}{4 \left( \epsilon_q^{(0)} - \epsilon_n^{(0)} \right)} \] 
(D.76)
The shift in the chemical potential \( \Delta \mu \) is given to second order by
\[ \Delta \mu = \Delta \mu^{(1)} + \Delta \mu^{(2)} \] 
(D.77)
where \( \Delta \mu^{(1)} \) and \( \Delta \mu^{(2)} \) are given respectively by (D.73) and (D.74). The energy shifts \( \Delta \epsilon_q \) are given to second order by
\[ \Delta \epsilon_q = \Delta \epsilon_q^{(1)} + \Delta \epsilon_q^{(2)} \] 
(D.78)
where \( \Delta \epsilon_q^{(1)} \) and \( \Delta \epsilon_q^{(2)} \) are given respectively by (D.75) and (D.76). We apply these results self-consistently by solving the GGPE (D.39), the shift in the chemical potential (D.77), the BdGEs (D.40) with the shifted chemical potential, viz.
\[ \epsilon_q \begin{bmatrix} u_q(\mathbf{r}) \\ v_q(\mathbf{r}) \end{bmatrix} = \int d\mathbf{r}' \begin{bmatrix} \left( \hat{\mathcal{L}}(\mathbf{r}, \mathbf{r}') - \Delta \mu \right) - \hat{\mathcal{M}}(\mathbf{r}, \mathbf{r}') - \left( \hat{\mathcal{L}}^*(\mathbf{r}, \mathbf{r}') - \Delta \mu \right) \end{bmatrix} \begin{bmatrix} u_q(\mathbf{r}') \\ v_q(\mathbf{r}') \end{bmatrix} \] 
(D.79)
and the energy shifts (D.78) self-consistently.
Appendix E

Two-state and Multi-state Models for Vortices in BECs

E.1 Two-state Model

Consider the two-state model presented in section 7.3.1 given by two-mode superposition states of the form [90, 105]

\[
\Phi(r, \theta, t) = \frac{1}{\sqrt{2\pi}} \left( a_g(t)\phi_g(r) + a_v(t)\phi_v(r)e^{i\theta} \right)
\]

(E.1)

where

\[
a_g(t) = a_g e^{-i\mu_g t} \\
a_v(t) = a_v e^{-i\mu_v t}
\]

(E.2)

We solve this by transforming to the rotating frame. In the rotating frame

\[
\hat{h}(r, \theta) \rightarrow \hat{h}_{\Omega}(r, \theta) = \hat{h}(r, \theta) + i\Omega \frac{\partial}{\partial \theta}
\]

(E.3)

so

\[
\hat{h}_l(r) \rightarrow \hat{h}_{\Omega,l}(r) = \hat{h}_l(r) - \Omega l
\]

(E.4)

In the co-rotating frame \(\theta \rightarrow \theta - \Omega t\), a stationary solution can be found, and the ansatz (E.1) becomes

\[
\Phi(r, \theta, t) = e^{-i\mu t}\Phi(r, \theta) = e^{-i\mu t} \frac{1}{\sqrt{2\pi}} \left( a_g \phi_g(r) + a_v \phi_v(r)e^{i\theta} \right)
\]

(E.5)

Here the chemical potential is given by

\[
\mu = \mu_g
\]

(E.6)
Appendix E. Two-state and Multi-state Models for Vortices in BECs

and the precessional frequency of the vortex by

\[ \Omega = \mu_v - \mu_g \]  

(E.7)

### E.1.1 The Coupled GGPEs in the Rotating Frame

In the frame rotating at the precessional frequency \( \Omega \), we obtain the coupled GGPEs

\[
\mu \phi_g = \left[ \hat{h}_{\Omega,0} + C_{2D}^R \left( n_{g0} |\phi_g|^2 + 2 n_{v0} |\phi_v|^2 + 2 \tilde{N}^{(0)} + \tilde{M}^{(0)} \right) \right] \phi_g + \frac{a_{v0}}{a_{g0}} C_{2D}^R \left( 2 \tilde{N}^{(1)} + \tilde{M}^{(-1)} \right) \phi_v
\]  

(E.8)

and

\[
\mu \phi_v = \left[ \hat{h}_{\Omega,1} + C_{2D}^R \left( n_{v0} |\phi_v|^2 + 2 n_{g0} |\phi_g|^2 + 2 \tilde{N}^{(0)} + \tilde{M}^{(-2)} \right) \right] \phi_v + \frac{a_{g0}}{a_{v0}} C_{2D}^R \left( 2 \tilde{N}^{(-1)} + \tilde{M}^{(1)} \right) \phi_g
\]  

(E.9)

where

\[
n_{g0} = |a_{g0}|^2
\]

\[
n_{v0} = |a_{v0}|^2
\]  

(E.10)

and where we have defined the quantities

\[
\tilde{N}_c^{(l)}(r) \equiv \int_0^{2\pi} \frac{e^{il\theta}}{\sqrt{2\pi}} n_c(r, \theta) d\theta,
\]

(E.11)

\[
\tilde{N}^{(l)}(r) \equiv \int_0^{2\pi} \frac{e^{il\theta}}{\sqrt{2\pi}} n(r, \theta) d\theta,
\]

(E.12)

and

\[
\tilde{M}^{(l)}(r) \equiv \int_0^{2\pi} \frac{e^{il\theta}}{\sqrt{2\pi}} \tilde{n}(r, \theta) d\theta.
\]

(E.13)

We show this as follows:

In the co-rotating frame

\[
(-\nabla^2 + V) \Phi = e^{-i\mu t} \frac{1}{\sqrt{2\pi}} \left( a_{g0} \hat{h}_{\Omega,0} \phi_g + a_{v0} e^{i\theta} \hat{h}_{\Omega,1} \phi_v \right)
\]

(E.14)

and

\[
|\Phi|^2 = \frac{1}{2\pi} \left( |a_{g0}|^2 |\phi_g|^2 + a_{g0} a_{v0} e^{i\theta} \phi_g \phi_v + a_{g0} a_{v0} e^{-i\theta} \phi_g \phi_v + a_{v0} a_{v0} |\phi_v|^2 \right)
\]

(E.15)

so noting that \( C_{2D}^R = C_{2D}/2\pi \), we obtain

\[
C_{2D} \left( |\Phi|^2 + 2\tilde{n} \right) \Phi = e^{-i\mu t} C_{2D}^R \left\{ \left( |a_{g0}|^2 |\phi_g|^2 a_{g0} \phi_g + 2 |a_{v0}|^2 |\phi_v|^2 a_{g0} \phi_g + 2 \tilde{n} a_{g0} \phi_g \right) \\
+ \left( |a_{v0}|^2 |\phi_v|^2 a_{v0} \phi_v + 2 |a_{g0}|^2 |\phi_g|^2 a_{v0} \phi_v + 2 \tilde{n} a_{v0} \phi_v \right) \exp(i\theta) \\
+ a_{g0}^2 a_{v0} \phi_g \phi_v \exp(-i\theta) + a_{g0} a_{v0}^2 \phi_g \phi_v \exp(2i\theta) \right\}
\]

(E.16)
Appendix E. Two-state and Multi-state Models for Vortices in BECs

\[ C_{2D} \tilde{m}(r, \theta, t) R = e^{i \mu t} C_{2D} R \tilde{m}(r, \theta, t) \left( a_{g0} \phi_g + a_{v0} \phi_v e^{-i \theta} \right) = e^{i \mu t} C_{2D} R \tilde{m}(r, \theta) \left( a_{g0} \phi_g + a_{v0} \phi_v e^{-i \theta} \right) \]  
\quad (E.17)

where we note that \( \tilde{m}(r, \theta, t) \) has phase \(-2i \mu t\) in order to satisfy the stationary condition for the GGPEs, ie.

\[ \tilde{m}(r, \theta, t) = e^{-2i \mu t} \tilde{m}(r, \theta) \]  
\quad (E.18)

Now by (E.2) and (E.5)

\[ \left( i \frac{d}{dt} \right) \phi_g = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} i \frac{\partial \Phi}{\partial t} d\theta \]

and

\[ \left( i \frac{d}{dt} \right) \phi_v = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{-i \theta} i \frac{\partial \Phi}{\partial t} d\theta \]

and since now (cf (E.2), (E.6) and (E.7))

\[ i \frac{d}{dt} a_g = \mu a_g \]  
\quad (E.19)

and

\[ i \frac{d}{dt} a_v = \mu a_v \]  
\quad (E.20)

in the co-rotating frame, we obtain the coupled GGPEs

\[ \mu \phi_g = \left[ \hat{h}_{\Omega,0} + C_{2D}^{R} \left( n_{g0} |\phi_g|^2 + 2n_{v0} |\phi_v|^2 + 2\tilde{N}(0) + \tilde{M}(0) \right) \right] \phi_g + \frac{a_{v0}}{a_{g0}} C_{2D}^{R} \left( 2\tilde{N}(1) + \tilde{M}(-1) \right) \phi_v \]  
\quad (E.21)

and

\[ \mu \phi_v = \left[ \hat{h}_{\Omega,1} + C_{2D}^{R} \left( n_{v0} |\phi_v|^2 + 2n_{g0} |\phi_g|^2 + 2\tilde{N}(0) + \tilde{M}(-2) \right) \right] \phi_v + \frac{a_{g0}}{a_{v0}} C_{2D}^{R} \left( 2\tilde{N}(-1) + \tilde{M}(-1) \right) \phi_g . \]  
\quad (E.22)

Let us define the operators \( \hat{F}_{g,\Omega}, G_g, \hat{F}_{v,\Omega}, \) and \( G_v \) for the frame rotating about the axis of symmetry at angular frequency \( \Omega \) given respectively by

\[ \hat{F}_{g,\Omega} \equiv \hat{h}_{\Omega,0} + C_{2D}^{R} \left( n_{g0} |\phi_g|^2 + 2n_{v0} |\phi_v|^2 + 2\tilde{N}(0) + \tilde{M}(0) \right) = \hat{F}_g \]  
\quad (E.23)

\[ G_g \equiv \frac{a_{v0}}{a_{g0}} C_{2D}^{R} \left( 2\tilde{N}(1) + \tilde{M}(-1) \right) \]  
\quad (E.24)

\[ \hat{F}_{v,\Omega} \equiv \hat{h}_{\Omega,1} + C_{2D}^{R} \left( n_{v0} |\phi_v|^2 + 2n_{g0} |\phi_g|^2 + 2\tilde{N}(0) + \tilde{M}(-2) \right) = \hat{F}_v - \Omega \]  
\quad (E.25)

and

\[ G_v \equiv \frac{a_{g0}}{a_{v0}} C_{2D}^{R} \left( 2\tilde{N}(-1) + \tilde{M}(-1) \right) \]  
\quad (E.26)

Then the GGPEs in the rotating frame can be rewritten in the matrix form

\[ \mu \begin{bmatrix} \phi_g \\ \phi_v \end{bmatrix} = \begin{bmatrix} \hat{F}_{g,\Omega} & G_g \\ G_v & \hat{F}_{v,\Omega} \end{bmatrix} \begin{bmatrix} \phi_g \\ \phi_v \end{bmatrix} \]  
\quad (E.27)
E.1.2 The BdGEs

We first note that we can write

\[ u_q(r, \theta, t) = e^{-i\mu t} u_q(r, \theta) \]  \hspace{1cm} (E.28)

and

\[ v_q(r, \theta, t) = e^{i\mu t} v_q(r, \theta) \]  \hspace{1cm} (E.29)

so that (E.18) is satisfied.

We expand the quasi-particle amplitudes in terms of the complete single-particle basis

\[ \{ \xi_{ln}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} | n = 0, 1, \ldots; l = 0, \pm 1, \ldots \} \]  \hspace{1cm} (E.30)

and write

\[ u_q(r, \theta) = \sum_{nl} c_{q, ln} \xi_{ln}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} = \sum_{l} u_q^{(l)}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} \]  \hspace{1cm} (E.31)

and

\[ v_q(r, \theta) = \sum_{nl} d_{q, ln} \xi_{ln}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} = \sum_{l} v_q^{(l)}(r) \frac{e^{i\theta}}{\sqrt{2\pi}}. \]  \hspace{1cm} (E.32)

The BdGE for \( u_q \) in the co-rotating frame is given by

\[ \epsilon_q u_q = \left( i \Omega - \mu + 2C_{2D}^R (|\Phi|^2 + \tilde{n}) \right) u_q + C_{2D}^R (\Phi^2 + \tilde{m}) v_q \]  \hspace{1cm} (E.33)

so

\[ \epsilon_q \sum_l u_q^{(l)}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} = \sum_l \left\{ i \Omega - \mu + 2C_{2D}^R (n_{g0} |\phi_g|^2 + a_{g0} a_{v0} e^{i\theta} \phi_g \phi_v + a_{g0} a_{v0} e^{-i\theta} \phi_s \phi_v + |a_{v0}|^2 |\phi_v|^2 + \tilde{n}) \right\} u_q^{(l)}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} + C_{2D}^R \left[ a_{g0}^2 \phi_g^2 + 2a_{g0} a_{v0} \phi_g \phi_v e^{i\theta} + a_{v0}^2 \phi_v^2 e^{2i\theta} + \tilde{m} \right] v_q^{(l)}(r) \frac{e^{i\theta}}{\sqrt{2\pi}} \} \]  \hspace{1cm} (E.34)

Therefore, multiplying by \( e^{-i\theta} / \sqrt{2\pi} \), and integrating over all \( \theta \), and defining the quantities

\[ \hat{\mathcal{L}}^{(u)}_{ll'} = \begin{cases} \hat{\Omega}_{l,l'} + 2C_{2D}^R \left( n_{g0} |\phi_g|^2 + n_{v0} |\phi_v|^2 + \tilde{N}^{(0)} \right), & l' = l \\ 2C_{2D}^R \left( a_{g0} a_{v0} \phi_g \phi_v + \tilde{N}^{(\pm 1)} \right), & l' = l \pm 1 \\ 2C_{2D}^R \tilde{N}^{(l'-l)} , & l' \notin \{l, l \pm 1\} \end{cases} \]  \hspace{1cm} (E.35)

and

\[ \hat{\mathcal{M}}^{(u)}_{ll'} = \begin{cases} C_{2D}^R \left( a_{g0}^2 \phi_g^2 + \tilde{M}^{(0)} \right), & l' = l \\ C_{2D}^R \left( 2a_{g0} a_{v0} \phi_g \phi_v + \tilde{M}^{(-1)} \right), & l' = l - 1 \\ C_{2D}^R \left( a_{v0}^2 \phi_v^2 + \tilde{M}^{(-2)} \right), & l' = l - 2 \\ C_{2D}^R \tilde{M}^{(l'-l)} , & l' \notin \{l, l - 1, l - 2\} \end{cases} \]  \hspace{1cm} (E.36)
we find that
\[
\epsilon_q u_q^{(l)} = \sum_{l'} \left( \hat{L}_{ll'}^{(u)} u_q^{(l')} + \hat{M}_{ll'}^{(u)} v_q^{(l')} \right).
\] (E.37)

The BdGE for \( v_q \) in the co-rotating frame is given by
\[
-\epsilon_q v_q = \left( \hat{h}_\Omega^* - \mu + 2C^{R}_{2D} \left( |\Phi|^2 + \bar{n} \right) \right) v_q + C^{R}_{2D} \left( \Phi^* + \bar{m} \right)^* u_q
\] (E.38)
so
\[
-\epsilon_q \sum_l v_q^{(l)}(r) e^{i\theta} = \sum_l \left\{ \left[ \hat{h}_\Omega^* - \mu + 2C^{R}_{2D} \left( n_{g0} |\phi_g|^2 + a_{g0} a_{v0} e^{i\theta} \phi_g \phi_v + a_{g0} a_{v0} e^{-i\theta} \phi_s \phi_v + |a_{v0}|^2 |\phi_v|^2 + \bar{n} \right) \right] v_q^{(l)}(r) e^{i\theta} \right\}.
\] (E.39)

So again, multiplying by \( e^{-i\theta}/\sqrt{2\pi} \), and integrating over all \( \theta \), and defining the quantities
\[
\hat{L}_{ll'}^{(v)} = \begin{cases} \hat{h}_\Omega - l + 2C^{R}_{2D} \left( n_{g0} |\phi_g|^2 + n_{v0} |\phi_v|^2 + \bar{N}(0) \right) & , l' = l \\ 2C^{R}_{2D} \left( a_{g0} a_{v0} e^{i\theta} \phi_g \phi_v + \bar{N}(\pm 1) \right) & , l' = l \pm 1 \\ 2C^{R}_{2D} \bar{N}(l'-l) & , l' \notin \{l, l \pm 1\} \end{cases}
\] (E.40)

and
\[
\hat{M}_{ll'}^{(v)} = \begin{cases} C^{R}_{2D} \left( a_{g0}^2 \phi_g^2 + \bar{M}(0) \right) & , l' = l \\ C^{R}_{2D} \left( 2 a_{g0} a_{v0} e^{i\theta} \phi_g \phi_v + \bar{M}(\pm 1) \right) & , l' = l \pm 1 \\ C^{R}_{2D} \left( a_{v0}^2 \phi_v^2 + \bar{M}(\pm 2) \right) & , l' = l + 2 \\ C^{R}_{2D} \bar{M}(l'-l) & , l' \notin \{l, l \pm 1, l + 2\} \end{cases}
\] (E.41)

we find that
\[
-\epsilon_q v_q^{(l)} = \sum_{l'} \left( \hat{L}_{ll'}^{(v)} v_q^{(l')} + \hat{M}_{ll'}^{(v)} u_q^{(l')} \right).
\] (E.42)

Defining the vectors \( \mathbf{u}_q \), and \( \mathbf{v}_q \) corresponding to the \( u_q^{(l)}(r) \) and the \( v_q^{(l)}(r) \) and the matrix operators \( \hat{L}_u, \hat{M}_u, \hat{L}_v, \) and \( \hat{M}_v \) corresponding to the \( \hat{L}_{ll'}^{(u)} \), the \( \hat{M}_{ll'}^{(u)} \), the \( \hat{L}_{ll'}^{(v)} \) and the \( \hat{M}_{ll'}^{(v)} \) respectively, we obtain the BdGEs
\[
\begin{bmatrix} \hat{L}_u & \hat{M}_u \\ -\hat{M}_v & -\hat{L}_v \end{bmatrix} \begin{bmatrix} \mathbf{u}_q \\ \mathbf{v}_q \end{bmatrix} = \epsilon_q \begin{bmatrix} \mathbf{u}_q \\ \mathbf{v}_q \end{bmatrix}.
\] (E.43)

We solve the two-state GGPE (E.27) and BdGEs (E.43) for various values of \( \alpha \) lying between 0 and 1 and for various values of \( a_g \) and \( a_v \) in the zero temperature limit.
E.2 Generalised Multi-state Model

We generalise the two-state model [90, 105], and write the following ansatz for the condensate wave function

$$\Phi(r, \theta, t) = e^{-i\mu t} \frac{1}{\sqrt{2\pi}} \left( a_g \sum_{l \neq 1} e^{-i\Omega l t} \phi_g^{(l)}(r)e^{il\theta} + a_v e^{-i\Omega t} \phi_v(r)e^{i\theta} \right). \quad (E.44)$$

Here we expand $\phi_g^{(l)}(r)$ and $\phi_v(r)$ in the single particle basis $\{\xi_n(r)\}$, i.e.

$$\phi_g^{(l)}(r) = \sum_n \alpha_{ln} \xi_n(r) \quad (E.45)$$

and

$$\phi_v(r) = \sum_n \alpha_{1n} \xi_n(r). \quad (E.46)$$

In the co-rotating frame $\theta \rightarrow \theta - \Omega t$, a stationary solution can be found in the rotating frame. We have, as before (E.3), (E.4)

$$\hat{h}(r, \theta) \rightarrow \hat{h}_\Omega(r, \theta) = \hat{h}(r, \theta) + i\Omega \frac{\partial}{\partial \theta}$$

so

$$\hat{h}(r) \rightarrow \hat{h}_\Omega, l(r) = \hat{h}_l(r) - \Omega l.$$  

E.2.1 The Coupled GGPEs

In the co-rotating frame $\theta \rightarrow \theta - \Omega t$ the ansatz (E.44) becomes (after cancellation of phase factors)

$$\Phi(r, \theta, t) = e^{-i\mu t} \Phi(r, \theta) = e^{-i\mu t} \frac{1}{\sqrt{2\pi}} \left( a_g \sum_{l \neq 1} \phi_g^{(l)}(r)e^{il\theta} + a_v \phi_v(r)e^{i\theta} \right) \quad (E.47)$$

So in the rotating frame, we have the time-independent GGPE

$$\mu \Phi = \left[ \hat{h}_\Omega + C_{2D}^R (n_c + 2\tilde{n}) \right] \Phi + C_{2D}^R \tilde{m} \Phi^*. \quad (E.48)$$

Substituting the ansatz (E.47) into the above, multiplying by $e^{-i\theta}/\sqrt{2\pi}$ and integrating over all $\theta$, we obtain the GGPE

$$\mu \phi_g^{(l)}(r) = \left[ \hat{h}_l - \Omega l \right]\phi_g^{(l)}(r) + C_{2D}^R \sum_{l' \neq 1} \left( N_c^{(l'-l)} + 2\tilde{N}^{(l'-l)} + \tilde{M}^{(l'-l)} \right) \phi_g^{(l')}(r) + \frac{a_v}{a_g} C_{2D}^R \left( N_c^{(l'-1)} + 2\tilde{N}^{(1-l)} + \tilde{M}^{(1-l)} \right) \phi_v(r) \quad (E.49)$$
for the radial ground state $\phi_g^{(l)}$, and multiplying by $1/\sqrt{2\pi}$, and integrating over all $\theta$, we obtain the GGPE

$$\mu \phi_v(r) = \left[ \hat{h}_1 - \Omega + C_{2D}^R \left( N_c^{(0)} + 2 \tilde{N}(0) + \tilde{M}^{(-2)} \right) \right] \phi_v(r)$$

$$+ 2 a_v C_{2D}^R \sum_{l' \neq 1} \left( N_c^{(l'-1)} + 2 \tilde{N}(l'-1) + \tilde{M}^{(-l'-1)} \right) \phi_g^{(l')}(r)$$

(E.50)

for the radial vortex state $\phi_v(r)$.

### E.2.2 Constraint equations for $\mu$ and $\Omega$

We first note the normalisation conditions

$$\sum_{l \neq 1} \int_0^\infty r dr \phi_g^{(l)}(r)^2 = 1 \quad (E.51)$$

and

$$\int_0^\infty r dr \phi_v^2(r) = 1. \quad (E.52)$$

Since the factors $a_g$, and $a_v$ also satisfy the normalisation condition

$$|a_g|^2 + |a_v|^2 = 1 \quad (E.53)$$

the normalisation condition

$$\int_0^{2\pi} \int_0^\infty r dr d\theta |\Phi(r, \theta)|^2 = \int_0^\infty r dr N_c^{(0)}(r) = 1 \quad (E.54)$$

is satisfied, as required.

Since

$$\hat{h}_1 \phi_g^{(l)}(r) = \sum_n \alpha_{ln} \mu_{SP}^{(l)} \xi_n(r) \quad (E.55)$$

multiplying both sides of (E.49) by $\phi_g^{(l)}(r)$, integrating over all $r$ and summing over all $l$, we find using the normalisation condition (E.51) the expression

$$\mu = \sum_{l_n \neq l} \alpha_{ln}^2 \mu_{SP}^{(l)} - \Omega \sum_{l_n \neq l} l \alpha_{ln}^2 + \sum_{l \neq l'} \frac{I_v^{(gg)}}{a_v} - \sum_{l \neq l'} I_{l'}^{(vg)}$$

(E.56)

for $\mu$, where we have defined the integrals

$$I_{l'}^{(gg)} \equiv C_{2D}^R \int_0^\infty r dr \left( N_c^{(l'-1)}(r) + 2 \tilde{N}(l'-1)(r) + \tilde{M}^{(-l'-1)}(r) \right) \phi_g^{(l')}(r) \phi_g^{(l)}(r)$$

(E.57)

and

$$I_{l'}^{(vg)} \equiv C_{2D}^R \int_0^\infty r dr \left( N_c^{(1-l)}(r) + 2 \tilde{N}^{(1-l)}(r) + \tilde{M}^{(-1-l)}(r) \right) \phi_v(r) \phi_g^{(l)}(r).$$

(E.58)
Since
\[ \hat{h}_1 \phi_v(r) = \sum_n \alpha_n \mu_S \xi_n^{(1)}(r) \] (E.59)
multiplying both sides of (E.50) by \( \phi_v(r) \) and integrating over all \( r \), we find that
\[ \mu = \sum_n \beta_n^2 \mu_S \xi_n^{(1)} - \Omega + I^{(vv)} + a_g/a_v \sum_{l \neq 1} I^{(gv)} \] (E.60)
where we have defined the integrals
\[ I_{l'}^{(gv)} \equiv C_{2D}^R \int_0^\infty rdr \left( N^{(l'-1)}(r) + 2 \tilde{N}^{(l'-1)}(r) + \tilde{M}^{(-l'-1)}(r) \right) \phi_{l'}(r) \phi_v(r) \] (E.61)
and
\[ I^{(vv)} \equiv C_{2D}^R \int_0^\infty rdr \left( N^{(0)}(r) + 2 \tilde{N}^{(0)}(r) + \tilde{M}^{(-2)}(r) \right) \phi_v^2(r). \] (E.62)
Here we have made use of the normalisation condition (E.52). We can simplify (E.56) and (E.60) by defining the quantities
\[ C_g \equiv \sum_{l,n,l \neq 1} l \alpha_l^2 \] (E.63)
\[ K_g \equiv \sum_{l,n,l \neq 1} \alpha_l^2 \mu_S \xi_n^{(1)} + \sum_{l,l' \neq 1} I^{(gg)}_{ll'} + a_g/a_v \sum_{l \neq 1} I^{(vg)}_l \] (E.64)
and
\[ K_v \equiv \sum_n \beta_n^2 \mu_S \xi_n^{(1)} + I^{(vv)} + a_g/a_v \sum_{l' \neq 1} I^{(gv)}_{l'}. \] (E.65)
Then, solving for \( \mu \) and \( \Omega \) we find that
\[ \mu = K_v - \frac{K_g - K_v}{C_g - 1} \] (E.66)
and
\[ \Omega = \frac{K_g - K_v}{C_g - 1}. \] (E.67)
Appendix F

Additional Simulations

F.1 Simulation of Stirring of the Condensate using Time-Dependent HFB in the G1 Approximation

We repeat simulation 3, i.e. a BEC stirred using a single Gaussian stirrer given by equation (7.87) for 4.5 trap cycles at stirring angular frequency $\Omega_s = 0.5\omega_r$ using the time dependent G1 approximation (c.f. equations (2.74)-(2.80)) given by the GGPE

$$i\hbar \frac{\partial}{\partial t} \Phi(r,t) = \left( \hat{h}(r) - \mu + g \left( |\Phi(r,t)|^2 + 2\tilde{n}(r,t) \right) \right) \Phi(r,t) + g\tilde{m}(r,t)\Phi^*(r,t)$$  \hspace{1cm} (F.1)

and the modified BdGEs given by

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} u_q(r,t) \\ v_q(r,t) \end{bmatrix} = \begin{bmatrix} \hat{L}_G(r,t) & \mathcal{M}_G(r,t) \\ -\mathcal{M}_G^*(r,t) & -\hat{L}_G^*(r,t) \end{bmatrix} \begin{bmatrix} u_q(r,t) \\ v_q(r,t) \end{bmatrix}$$  \hspace{1cm} (F.2)

where

$$\hat{L}_G(r,t) \equiv \hat{h}(r) - \mu + 2g \left( |\Phi(r,t)|^2 + \tilde{n}(r,t) \right) + 2g\tilde{m}(r,t) |\Phi(r,t)|^2 / \Phi^2(r,t)$$

$$\mathcal{M}_G(r,t) \equiv U_c(r,t)\Phi^2(r,t)$$  \hspace{1cm} (F.3)

We re-write $\hat{L}_G(r,t)$ as

$$\hat{L}_G(r,t) = \hat{h}(r) - \mu + 2g \left( |\Phi(r,t)|^2 + \tilde{n}(r,t) \right) + 2g\tilde{m}(r,t) \exp(-2i\chi(r,t))$$  \hspace{1cm} (F.4)

where

$$\chi(r,t) \equiv \arctan \left( \frac{\text{Im} \left( \Phi(r,t) \right)}{\text{Re} \left( \Phi(r,t) \right)} \right)$$  \hspace{1cm} (F.5)

which is preferable numerically as it avoids possibilities of divergence of the wave-functions. Inspection of figure F.1, which shows the condensate, the thermal and the total angular
Appendix F. Additional Simulations

Figure F.1: (Colour on-line) Stirring of condensate showing (a) $z$-component of total angular momentum (solid black line), condensate angular momentum (dashed blue line), and thermal population angular momentum (dash-dotted red line) versus time, (b) change in thermal population $\Delta N_t(t) - \Delta N_t(0)$ versus time, (c) change in condensate population $\Delta N_c(t) - \Delta N_c(0)$ versus time, and (d) change in total population $\Delta N(t) - \Delta N(0)$ showing the violation of number conservation. The condensate is stirred at frequencies $0.5\omega_r$ for 4.5 trap cycles using a single Gaussian stirrer situated at at $a = 1.5r_0$ off axis, are of amplitude $10\hbar\omega_r/2$, FWHM $0.82r_0$, and are switched on adiabatically over 0.2 trap cycles. The change in the populations $\Delta N_t$ and $\Delta N_c$ are given in units of $N$. All angular momenta are in units of $N\hbar$. 

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Figure F.2: Stirring of condensate using a Gaussian stirrer at stirring frequency $0.5\omega_r$ for 4.5 trap cycles (a) x-displacement of vortex 1, (b) y-displacement of vortex 1, and (c) trajectory of vortex 1 over a period of ten trap cycles (d) x-displacement of vortex 2, (e) y-displacement of vortex 2, and (f) trajectory of vortex 2 over a period of ten trap cycles. All Gaussian stirrers are situated at $a=1.5r_0$ off axis, are of coupling strength $10\hbar\omega_r/2$, FWHM $0.82r_0$, and are switched on adiabatically over 0.2 trap cycles. All positions are in units of the harmonic oscillator length $r_0$.

momentum $L_z$ versus time, and the changes in the thermal, condensate and total populations as a function of time clearly reveals that both number and angular momentum conservation are violated, in contrast to the time-dependent HFB simulations (see figure 7.15) which demonstrates that these quantities are conserved. However, in spite of this serious defect, figure F.2 shows that two vortices are still produced (c.f. figure 7.17), and that the vortex trajectories shown in figure F.3. are still quite similar to those shown in figure 7.19 II.

F.2 Perturbation Results for a BEC in the absence of Vortices

Perturbation calculations using the perturbation scheme defined by equations (4.145)-(4.152) have been performed for a BEC in the absence of any vortices for a mode cut-off of 209, and are presented in figure F.4. We note that the energy spectrum is slightly over-corrected (by $\sim 1\%$), but this over-correction is not systemic as can be seen in figure F.5 which shows the higher quasi-particle excitation energies $\epsilon_4 \rightarrow \epsilon_9$. We note also from figure F.4 (e) that the thermal densities in the HFB simulations performed here are
Figure F.3: Simulated absorption images [116] - stirring of condensate in an anti-clockwise direction using one Gaussian stirrer at $a = 1.5 r_0$ off axis, of amplitude $10 \hbar \omega_r/2$, FWHM $0.82 r_0$, switched on adiabatically over 0.2 trap cycles, stirring frequency $0.5 \omega_r$, stirrer on for 4.5 trap cycles after (a) 0.5, (b) 1, (c) 1.5, (d) 2, (e) 2.5, (f) 3, (g) 3.5, (h) 4, (i) 4.5, (j) 5, (k) 5.5, (l) 6, (m) 6.5, (n) 7, (o) 7.5, (p) 8, (q) 8.5, (r) 9, (s) 9.5, and (t) 10 trap cycles. All positions are in units of the harmonic oscillator length $r_0$. 
Figure F.4: (Colour on-line) Perturbed excitation energies and thermal populations showing the (a) Kohn mode (m=1), (b) the m=2, and (c) the m=0 excitation energies versus temperature, (d) first three excitation energies i.e. the m=1, m=2 and m=0 versus temperature, and (e) the thermal population versus temperature for first-order perturbed orthogonal HFB (red triangles), for second-order perturbed orthogonal HFB (black circles), HFB Popov (black diamonds), and orthogonal HFB Popov (black squares). In panel (e) the thermal population is also shown for (non-perturbed) orthogonal HFB (downward black triangles). All energies are in trap units $\hbar \omega_t$, and populations in units of $N$. 


Figure F.5: (Colour on-line) Perturbed excitation energies showing the (a) \( q=4 \), (b) \( q=5 \), (c) \( q=6 \), (d) \( q=7 \), (e) \( q=8 \), and (f) \( q=9 \) excitation energies versus temperature for first-order perturbed orthogonal HFB (red triangles), for second-order perturbed orthogonal HFB (black circles), HFB Popov (black diamonds), and orthogonal HFB Popov (black squares). In panel (e) the thermal population is also shown for (non-perturbed) orthogonal HFB (downward black triangles). All energies are in trap units \( \hbar \omega_r \).
Figure F.6: (a) Precessional frequency $\Omega$ (in units of radial trapping frequency $\omega_r$) versus vortex position $a$ at temperatures 0nK, 2nK, 5nK and 7.5nK (triangles, diamonds, circles, squares respectively), (b) Precessional frequency $\Omega$ versus temperature $T$ at vortex positions 0.1, 0.5, 0.8 and 1.1 (triangles, diamonds, circles, squares respectively), (c) LCLS energy $\epsilon_{LCLS}$ versus vortex position $a$ at temperatures 0nK, 2nK, 5nK and 7.5nK (triangles, diamonds, circles, squares respectively), (d) LCLS energy $\epsilon_{LCLS}$ versus temperature $T$ at vortex positions 0.1, 0.5, 0.8 and 1.1 (triangles, diamonds, circles, squares respectively). All distances are in harmonic oscillator units $r_0$, frequencies in units $\omega_r$, and energies in trap units $\hbar \omega_r$. 
under-estimated by \( \lesssim 10\% \) as alluded to earlier towards the end of chapter 4, but that this should not qualitatively affect the results here.

### F.3 The Effect of the Projection Operator \( \hat{P}(r, r', t) \) in the GGPE in Orthogonal HFB on the Precession of Off-Axis Vortices

The finite temperature time-independent calculations for off-axis vortices of section 7.4.3 in chapter 7 were repeated, now including the projection operator \( \hat{P}(r, r', t) \) in the GGPE (4.106)

\[
\Delta \mu \Phi(r) = \left( \hat{h}(r) - \mu + g (|\Phi(r)|^2 + 2\bar{n}(r)) \right) \Phi(r) + g \bar{m}(r) \Phi^*(r) - \int dr' \hat{P}(r', r) \Phi(r')
\]  

(F.6)

in Orthogonal HFB equations (4.106), (4.107), and the results presented in figure F.6. Comparing figures 7.5 and F.6 we notice that the results are quite similar for low \( T \), but exhibit an upward shift of \( \sim 5-10\% \) for higher temperatures.