Dipolar Bose-Einstein Condensate with a Vortex

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Abstract

We theoretically consider the properties of a dipolar Bose-Einstein condensate with a vortex. Our theory includes the influence of the leading order quantum fluctuation corrections which allows the condensate to stabilize into a droplet state in the regime of dominant dipole interactions. We develop numerical techniques to accurately and efficiently calculate the stationary vortex states and the quasi-particle excitations. These methods are carefully benchmarked where possible.

We make a brief study of self-bound vortex droplets, considering their basic properties, and presenting a phase diagram for where they exist. We also compare our calculations to results which appeared from another group during our research. We show that their results suffer from serious numerical issues and are unreliable.

We focus on studying the properties of a vortex line in an elongated dipolar Bose-Einstein condensate confined by a prolate trap. Increasing the strength of the dipole-dipole interactions relative to the short ranged contact interactions we find that the system crosses over to a self-bound vortex droplet stabilized from collapse by quantum fluctuations. We calculate the quasiparticle excitation spectrum of the vortex state, which is important in characterizing the vortex response, and assessing its stability. When the DDIs are sufficiently strong we find that the vortex is dynamically unstable to quadrupolar modes.
Acknowledgements

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Chapter 1

Introduction

1.1 Bose-Einstein Condensate

A Bose-Einstein condensate (BEC) is a phase of matter in which indistinguishable bosons condense into a single particle state. It was predicted by Bose and Einstein in the early 20th century, but required extraordinary low temperatures (approaching absolute zero) to occur. With the development of laser [1–3] and evaporative [5–7] cooling of atomic gases the first BECs were produced in 1995 with the alkali atoms rubidium, sodium and lithium [8–10] [see Fig. 1.1].

Figure 1.1: The velocity distributions associated with the first BEC produced by the group at JILA using rubidium-87 in 1995. From left to right the subplots have temperatures of about 400nK, 200nK and 50nK, respectively. While the critical temperature for condensation here is estimated to be 200nK. The sharp anisotropic central spike in the velocity distribution in the lower temperature cases reveals the condensate, while the isotropic background is the non-condensed “thermal cloud”. (Figure taken from [11])
A wide range of physics has been explored with BECs. For example studies of superfluidity [12], including the production and characterization of quantized vortices [13]. Also studies of single particle and many-body dynamics [14] using the BEC as a source of highly coherent and low entropy matter waves. A key feature of these systems is the simple and well characterized interaction between the atoms.

For the case of the alkali atoms the interactions are completely described in the low temperature regime as a contact interaction with a strength determined by the $s$-wave scattering length. The ability to control the $s$-wave interaction using Feshbach resonances has allowed experiments to dynamically change how the condensed particles interact and opened the door to many interesting lines of investigation.

1.2 Dipolar Condensates and Droplets

It is of interest to have cold-atomic systems with longer-ranged interactions than the contact interaction. For neutral atoms the longest range interaction permissible is the dipole-dipole interaction (DDI). This can be realized in atoms that have a large (ground state) magnetic moment. The first atom with an appreciable magnetic moment to be successfully cooled into a BEC was chromium-52 by the experimental group in Stuttgart in 2005 [15]. This system was able to preform some initial studies showing the effects of DDI on BECs [15–18] [e.g. see Fig. 1.2].

More recently (c. 2012) the lanthanides dysprosium [19, 20] (the most magnetic atom) and erbium [21] were Bose condensed. The favourable properties of the lanthanides, including their large DDI, have generated a lot of interest in so called dipolar BECs, and have led to a number of important observations. For example, the observation of interaction induced roton excitations [22] and anisotropic critical velocity [23].

In 2016 a newly commissioned dysprosium experiment at Stuttgart made an unexpected observation [24]. The experiment prepared a dysprosium condensate in a regime where it was expected to be mechanically unstable to collapse. Normally an unstable BEC undergoes rapid and violent dynamics resulting in significant heating and atom loss through three-body recombination (e.g. see [25–27]). Instead this experiment, aided by high-resolution in situ imaging, noticed that the condensate formed into an array of stable long-lived ($\sim 300$ ms) droplets that organized themselves into an approximately triangular lattice [see Fig. 1.3]. The experiment termed this phenomenon as the Rosensweig instability of a quantum ferrofluid, drawing analogy to the Rosenweig instability of a classical ferrofluid [see Fig. 1.4].

A lot of interest has surrounded the physical mechanism leading to the formation of stable droplets. Subsequent theory and experiments have established that the collapse, being driven by attractive DDI, is arrested by an effective repulsive force arising from
quantum fluctuations \cite{29,33}. The leading order effects of quantum fluctuations on the energy of a dilute BEC were first described by the Lee, Huang, and Yang in 1957 \cite{34,35} and their result is often referred to as the LHY-term. The LHY term is normally quite small and difficult to measure in BECs, but as the droplets are appreciably more dense (i.e. $n_{\text{BEC}} \sim 10^{20} \text{ cm}^{-3}$ and $n_{\text{droplet}} \sim 10^{21} \text{ cm}^{-3}$), then the LHY term is important.

It was also realized that for sufficiently many atoms a droplet could become self-bound and exist as a localized matterwave in the absence of any confining potential \cite{36} [see Fig. 1.5]. This prediction was observed by the Stuttgart group later in 2016 \cite{37} [see Fig. 1.6], where the droplet was seen to cohere together for up to $\sim 100$ ms after the trapping potential was removed. Ultimately the droplet evaporates (falls apart) when the number of atoms within it decays below a critical number due to three-body recombination (the dominant atom loss mechanism).
Figure 1.3: (a) Schematic of the experiment: a stable oblate condensate is prepared then the relative strength of the DDIs ($\epsilon_{dd}$) is increased and an array of droplets forms. (b) *in situ* images of the droplet arrays formed in the experiment. The number of droplets increases across these subplots from 2 to 10 as the atom number in the initial condensate is increased. There is approximately $\sim 10^3$ atoms per droplet, and their lifetime is $\gtrsim 100$ ms (Figure taken from [24]).

There has been considerable experimental and theoretical activity exploring the properties of droplets such as their collective modes [32, 38, 30, 39], and methods to controllably produce single droplets [30, 33] and multiple droplet arrays [40, 41]. We also note that two component (or binary) condensates of non-dipolar atoms have been used to produce droplets [42, 43]. In these experiments the two components were different spin-states of potassium-39, and the droplets formed when the interspecies contact interaction was tuned sufficiently attractive.
Figure 1.4: Typical Rosensweig instability of a ferrofluid (colloidal liquids of nanoscale ferromagnetic particles suspended in a carrier fluid) induced by an external magnetic field. (Figure taken from [28])

Figure 1.5: Numerical simulation of the process to prepare a self-bound droplet from a trap bound dysprosium condensate. Black lines indicate contours of the harmonic trap, and colours indicate density isosurfaces of the condensate. The s-wave scattering length \( a_s \) is reduced over 10 ms to bring the system into the (unstable) dipole dominated regime where a self-bound droplet forms. Subsequently the trap is turned off and the droplet is seen to cohere. (Figure taken from [36])
Figure 1.6: (a) Experimental images of self-bound droplets. Here the droplet (imaged taken down the long axis) is not confined by a trap but is levitated by a gradient field to avoid it accelerating due to gravity. The left hand side subplots are for a self-bound droplet starting with a larger atom number than the sequence on the right hand side. Eventually, due to atom loss, the droplets get too small and evaporate (unbind). (b) The survival probability histogram of a droplet presented as function of levitation time with different colours denoted different magnetic field (used to control the short range interaction strength). (Figure taken from [37])

1.3 Work of this Thesis: Vortices in Dipolar BECs and Droplets

1.3.1 Motivation

In late 2017 a preprint appeared on the arXiv by Cidrim et al. [44] reporting theoretical results for vortices in a self-bound dipolar droplet. In particular dipolar droplets tend
to elongate in the direction along which the dipoles are polarized, and they considered the case of a vortex line extending along this axis. They found that these vortex droplets usually decayed very rapidly through a dynamic instability, breaking up into two filaments and ejecting the vortex core [see Figs. 1.7(a)-(c)]. Significantly they predicted that these vortex droplets could become stable for large atom numbers and relatively strong DDIs [see Figs. 1.7(d)-(f)]. The majority of this paper was concerned with stationary states obtained from extended meanfield calculations. These calculations extend the standard Gross-Pitaevskii theory for a dipolar condensate by adding a local density treatment of the LHY term. Conclusions about the vortex stability were made by comparing the energy of a vortex droplet to two non-vortex droplets each with half the atom number. Some dynamic calculations [i.e. those shown in Fig. 1.7] were shown that supported these conclusions.

Figure 1.7: Dynamical simulation of self-bound droplet with a vortex contained in the work of Cidrim et al. [44]. Subplots (a)-(c) show the time evolution for a vortex droplet $N = 10^4$ atoms and inverse relative dipole strength of $\epsilon_{dd}^{-1} = 0.2$. Subplots (d)-(f) show the evolution for a droplet with $N = 10^5$ and inverse relative dipole strength $\epsilon_{dd}^{-1} = 0.1$. Here $t_0 = ma_{dd}/\hbar$ is the computational time unit. (Figure taken from [44])

Existing comparisons between extended meanfield theory and experimental work with dipolar droplets (without vortices) indicate that this theory should be reliable, at least for the regime where the DDIs are not too strong relative to the contact interactions. However, the results presented in the preprint appeared to suffer from some serious technical issues indicating that their numerical solutions were highly unreliable. For example, properties such as the widths and energies of the droplets did not vary smoothly with the interaction parameter and displayed a high degree of scatter on a log-scale. Accurate calculations for dipolar BECs are notoriously difficult because of the singular form of the long-ranged and anisotropic DDI. Regularization techniques have been developed to improve the convergence of the DDI calculations, but these are
difficult to apply in highly asymmetric regimes (like in droplets) and in no mention is made of using such techniques.

The initial motivation of this research was to improve on the Cidrim et al. results by developing appropriate numerical techniques to obtain accurate self-bound vortex droplet solutions. In our results we found that the primary conclusion of Cidrim et al. was incorrect, i.e. their prediction of energetically stable vortex droplets was the result of inaccurate calculations. In the meantime Cidrim et al. significantly revised their paper, improving some of their results, and removing the erroneous conclusion. Their manuscript was published in late 2018 as Ref. [45].

However, many important issues remain about vortices in dipolar BECs and droplets, and serve as the motivation for our work:

- The dynamical simulations [e.g. see Figs. 1.7(a)-(c)] reveal a rapid decay of the vortex. Most likely this is associated with a dynamic instability (unstable excitation) rather than an energetic instability.

- To date in the 14 years since dipolar BECs have been first produced there has never been a direct experimental observation of a vortex in this system (in either condensate or droplet regime). In comparison for BECs with contact interactions there has been an extensive array of investigations of vortex properties [46].

### 1.3.2 Our Work

Here our primary aim is to develop methods and understanding of a vortex line in an elongated dipolar BEC. We present the basic formalism of dipolar BECs with quantum fluctuations in chapter 2, including both the extended meanfield theory to describe the condensate and the Bogoloibov-de Gennes equations for the condensate excitations. In Chapter 3 we introduce the numerical techniques we have developed to solve for the vortex stationary states and the excitations. This chapter represents the majority of the technical work executed in this research and where the most significant amount of research time was invested. In particular the BdG solutions are extremely challenging in the regime of elongated condensates with DDIs, and our results are the first of their kind. In Chapter 4 we present results for the stationary states of self-bound vortex droplets, showing their basic properties and the phase diagram of parameters where they should exist. We also make a critical comparison to the results of Ref. [45]. Chapter 5 represents the main result of this thesis. We study the cross over of an elongated systems with a vortex from a condensate (at weak relative DDIs) to a vortex droplet (at stronger DDIs). Our analysis involves understanding both the stationary solutions and spectrum of excitations. We are able to identify the Kelvin wave (helical) excitations of the vortex line and that quadrupolar modes lead to the fundamental
splitting instability seen in the regime of stronger DDIs (i.e as the system approaches becoming a self bound droplet).

The work in chapter 5 was published in December 2018 as [47]:


The extensive development of numerical methods in Chapter 3 is currently being prepared for publication.
Chapter 2

Formalism

In this chapter we introduce the main formalism we will use for the calculations in the remainder of this thesis. First, we discuss the main types of interaction in our system. We focus solely on neutral atoms, so the most significant interactions are the van der Waals interaction and the dipole-dipole interaction (DDI). Next, we discuss the Gross-Pitaevskii equation which describes the stationary states of the system, and the variational method which gives some intuition about the system. Finally, we linearise the excitations and develop the Bogoliubov-de Gennes equations, which will be useful to study the dynamics of our system.

2.1 Contact Interaction

The van der Waals interaction is isotropic and short ranged with the interaction proportional to $r^{-6}$ for large $r$. For our low temperature gases, we consider low $k$ interactions, where $k$ is the wave vector of the interaction in momentum space and $k = |k|$. The partial-wave scattering phase shifts for rotational quantum number $l$ are proportional to a power of $k$. For the van der Waals interaction, the phase shift is linear for $s$-waves ($l = 0$) and a higher power of $k$ for $l > 0$. So, we restrict ourselves to $s$-wave interaction, for which the zero energy limit is given by

$$U_s(r) = g_s \delta(r),$$  \hspace{1cm} (2.1)

where $r = \mathbf{x} - \mathbf{x}'$ with $\mathbf{x}$ and $\mathbf{x}'$ being the positions of the two interacting particles, $g_s = 4\pi\hbar^2a_s/M$ is the $s$-wave coupling constant, $a_s$ is $s$-wave scattering length, and $M$ is the mass of particle.
2.1.1 Tuning the Contact Interaction with a Feshbach Resonance

By using a Feshbach Resonance, one can tune the scattering length of the interaction. This works by using the bound-state in a closed channel to couple with atoms colliding in an open channel. Then, by applying external magnetic field to tweak the closed channel bound state, the desired scattering length of the s-wave interactions in the system can be achieved. Fig. 2.1 gives a simplified demonstration of the procedure of the Feshbach resonance for a two body system.

![Diagram](Figure 2.1: Basic model for the Feshbach resonance technique, here $R$ is $r$ in our notation. Figure taken from [48].)

2.2 Dipole-Dipole Interaction

In contrast to the contact interaction, the dipole-dipole interaction is long-ranged. If we have two dipoles pointing in the directions $e_1$ and $e_2$ as showed in Fig. 2.2(a), we can write the interaction potential as

$$U_{dd}(r) = \frac{3g_{dd}}{4\pi} (e_1 \cdot e_2)r^2 - 3(e_1 \cdot r)(e_2 \cdot r) \frac{1}{r^5},$$

(2.2)

where for a system of magnetic atoms

$$g_{dd} \equiv \frac{\mu_0 \mu^2}{3}$$

(2.3)
with $\mu_0$ the permeability of vacuum, and $\mu_m$ the permanent magnetic dipole moment of the particle, which is shown for a selection of atoms in Table 2.1. Note that the dipolar interaction strength $g_{dd}$ in Eq. (2.3) depends on the square of $\mu_m$, so that a factor of ten increase in the magnetic moment leads to a hundred-fold increase in the dipolar interaction strength.

![Image](image1.png)

Table 2.1: Magnetic dipole moment and dipole length of selected isotopes. Here $\mu_B$ is Bohr magneton and $a_0$ is Bohr radius. Data is from [49–51, 20, 21].

<table>
<thead>
<tr>
<th>Species</th>
<th>$\mu_m/\mu_B$</th>
<th>$a_{dd}/a_0$</th>
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<tr>
<td>$^{87}\text{Rb}$</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$^{52}\text{Cr}$</td>
<td>6</td>
<td>15</td>
</tr>
<tr>
<td>$^{168}\text{Er}$</td>
<td>7</td>
<td>66</td>
</tr>
<tr>
<td>$^{164}\text{Dy}$</td>
<td>10</td>
<td>131</td>
</tr>
</tbody>
</table>

We can define a dipole length $a_{dd}$ such that the DDI coupling constant $g_{dd}$ is given by

$$g_{dd} = \frac{4\pi a_{dd}\hbar^2}{M}.$$  \hspace{1cm} (2.4)

By use of a strong magnetic field along $z$-axis, we assume that all of the dipoles are

![Diagram](image2.png)

Figure 2.2: Two particles interacting with each other by the dipole-dipole interaction. (a) Different polarization for each of the particles. (b) Same direction of polarization for both of the particles. (c) Head-to-tail particles repel each other outward. (d) Side-by-side particles attract each other. (Figure taken from [51])
aligned in the z direction, so that Eq. (2.2) simplifies to

\[ U_{dd}(r) = \frac{3g_{dd}}{4\pi} \frac{1 - 3\cos^2 \theta}{r^3}, \]  

(2.5)

where \( \theta \) is the angle between the polarised direction of the dipoles and the direction vector between the dipoles, as shown in Fig. 2.2(b). The DDI is attractive when the atoms are side by side and repulsive when head to tail [see Figs. 2.2(c) and (d)].

### 2.2.1 Tuning the Dipole-Dipole Interaction

By applying rotating magnetic field [see Fig. 2.3] with a frequency higher than the chemical potential [which will be given in Eq. (2.13)] and lower than Larmor frequency one can tune the DDI strength, with the effective interaction given by the time average of the DDI. It has been predicted by [52] that the procedure will encounter difficulty due to dynamical instability, notwithstanding experimented success reported by [53], so further research on this is needed. The time-averaged DDI is

\[ \langle U_{dd}(r, t) \rangle = \frac{3g_{dd}}{4\pi} \frac{1 - 3\cos^2 \theta}{r^3} \left( \frac{3\cos^2 \varphi - 1}{2} \right). \]  

(2.6)

Figure 2.3: Rotating dipoles with frequency \( \Omega \), and \( \varphi \) being the angle of rotation from the z-axis. Figure taken from [51].

From this equation we can see the dipoles can be tuned by a factor of between 1 and \(-\frac{1}{2}\) times of the particle’s DDI strength, and it is dependent on the tilt angle \( \varphi \).
2.3 Gross-Pitaevskii Equation

In the previous section we introduced two body interactions. We combine Eq. (2.1) and Eq. (2.5) together in the form

$$U(r) = g_s\delta(r) + U_{dd}(r), \tag{2.7}$$

which includes all of the two-body interactions we consider in this thesis. In the meanfield approximation we assume a pure condensate, with all atoms having the same wavefunction \(\Psi(x)\). We can then identify stationary solution \(\Psi_c(x)\), by requiring \(\delta E[\Psi] / \delta \Psi = 0\) where \(E[\Psi]\) is the energy functional [see Eq. (2.12) below]. This gives the time-independent Gross-Pitaevskii equation (GPE) with the form

$$\mu \Psi_c(x) = \hat{L}_{\text{GP}} \Psi_c(x), \tag{2.8}$$

where

$$\hat{L}_{\text{GP}} = -\frac{\hbar^2}{2M} \nabla^2 + V_tr + \int dx'U(x - x')|\Psi_c(x')|^2 + \gamma_{\text{QF}} |\Psi_c(x)|^3 \tag{2.9}$$

\(\gamma_{\text{QF}} = \frac{32}{3} g_s \sqrt{\frac{a_s^3}{\pi}} \left( 1 + \frac{3}{2} \epsilon_{dd}^2 \right) \tag{2.10}\)

The details about the Quantum fluctuation (QF) term \(\gamma_{\text{QF}}\) will be discussed in Sec. 2.3.1 and \(\epsilon_{dd} = a_{dd}/a_s\) is the relative strength between dipole-dipole and contact interactions. Here \(\Psi_c\) is the condensate (meanfield) wavefunction and \(\mu\) is the condensate chemical potential.

We assume that a harmonic potential trap is used to confine the condensate, of the form

$$V_tr = \frac{1}{2} M(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \tag{2.11}$$

where \(\omega_{x,y,z}\) are trap frequencies in the direction of \(x, y\) and \(z\) axis, respectively. By summing up each component of the energy (i.e. kinetic, trap, contact, dipole, and QF energy) we then obtain the equation for total energy of the system with the form

$$E[\Psi] = E_K + E_V + E_C + E_D + E_{QF} \tag{2.12}$$

$$= -\frac{\hbar^2}{2M} \int dx \Psi^*(x) \nabla^2 \Psi(x) + \int dx V_tr(x)|\Psi(x)|^2 + \frac{g_s}{2} \int dx |\Psi(x)|^4$$

$$+ \frac{1}{2} \int dx \left[ \int dx'U_{dd}(x - x')|\Psi(x')|^2 \right] |\Psi(x)|^2 + \frac{2}{5} \int dx \gamma_{QF} |\Psi(x)|^5$$

where the terms in the second line are in the same order as in the first line of the
equation. We can calculate the chemical potential as

$$\mu = \frac{(E_K + E_V + 2E_D + 2E_C + 5E_{QF}/2)}{N},$$

(2.13)

where $N$ is the number of condensate atoms $N = \int d\mathbf{x}|\Psi_c|^2$. There are several ways to obtain stationary states of the GPE [see Eq. (2.8)], we will discuss the details in Ch. 3.

### 2.3.1 Quantum Fluctuations

The GPE meanfield theory is derived for the case of atoms in a product state, i.e. it is assumed that all atoms are in the same quantum state: the GPE wavefunction. However, even at zero temperature, the excitations of the GPE are occupied due to quantum (vacuum) fluctuations, giving rise to a ‘quantum depletion’. Corrections due to quantum fluctuations for a uniform gas with only contact interactions were calculated in 1957 by Lee, Huang and Yang (LHY) \[54, 35\]. In 2011 quantum fluctuations were calculated include dipolar interactions \[55, 56\], finding the results

$$\Delta E = \frac{2V}{5} \gamma_{QF} n^{5/2},$$

(2.14)

$$\Delta \mu = \frac{\partial \Delta E}{\partial N} = \gamma_{QF} n^{3/2},$$

(2.15)

for the energy and chemical potential corrections. Here $V$ is volume of the system, $N$ is number of particles, $n = N/V$ is density through out the system and

$$\gamma_{QF} \equiv \frac{32g_s}{3} \sqrt{\frac{a_3}{\pi}} Q_5(\epsilon_{dd}),$$

(2.16)

with $Q_5$ given as

$$Q_5(\epsilon_{dd}) = \frac{(3\epsilon_{dd})^{5/2}}{48} \left[ (8 + 26y + 33y^2)\sqrt{1+y} + 15y^3 \ln\left(\frac{1 + \sqrt{1+y}}{\sqrt{y}}\right) \right]$$

(2.17)

$$= 1 + \frac{3}{2} \epsilon_{dd}^2 + \mathcal{O}(\epsilon_{dd}^4)$$

(2.18)

$$y = (1 - \epsilon_{dd})/3\epsilon_{dd}.$$

(2.19)

While not strictly valid for $\epsilon_{dd} > 1$, the approximation given by Eq. (2.18) is surprisingly good for $\epsilon_{dd} \gtrsim 1$ as seem in Fig. 2.4 and we use that approximation throughout this thesis.

For our inhomogeneous system, we include quantum fluctuations by adjusting the chemical potential using the result from homogeneous case in the local density approx-
Figure 2.4: (a) Real part of both original $Q_5$ and the approximation Eq. (2.18) we used, in blue and orange dash, respectively. (b) The percentage difference between $Q_5$ and Eq. (2.18).
imation, i.e. using \( n \rightarrow n(x) = |\Psi_c(x)|^2 \) to give

\[
\Delta \mu(x) = \gamma_{\text{QF}}|\Psi_c(x)|^3. \tag{2.20}
\]

The function \( Q_5(\epsilon_{dd}) \) is an integral over wavevector \( k \). The result has a small imaginary part for \( \epsilon_{dd} > 1 \) due to the inclusion of small \( k \) (long wavelength) modes. Our system is finite sized, so inclusion of such long wavelength modes is unphysical. Using a small \( k \) cutoff in the integral can remove the imaginary part and does not significantly affect the real part \[33\].

In many cases quantum depletion is insignificant and can be ignored. However, without considering quantum fluctuations, a dipolar gas with sufficiently high \( \epsilon_{dd} \) is unstable by collapsing, due to the attractive component of the interaction (the homogeneous system is unstable for \( \epsilon_{dd} > 1 \)). The power of the wavefunction in the quantum fluctuation term is greater than the power on wavefunction for the two-body interaction terms in Eq. \[2.9\], so quantum fluctuations become more important in the regime of high density and are able to arrest the collapse. In 2016 [24], experiments observed the formation of the droplet crystal in a dipolar gas, this would not be possible in the GPE approximation (i.e. without the QF term).

### 2.4 Variational Method

By the variational principle we find an upper bound on the energy of the stationary state of the system. Although one can obtain a more accurate stationary state by solving the GPE, the variational method is much less time expensive. Also, if the variational results qualitatively agree with GPE, insight can be gained from looking at the analytical form of the variational energy.

#### 2.4.1 Variational Ansatz

For simplicity, we use a Gaussian ansatz with a vortex of charge \( s \)

\[
\psi_{\text{var}}^s(\rho, \phi, z) = \sqrt{N}\psi_{\text{var}}^s(\rho, \phi)\psi_{\text{var}}(z) \tag{2.21}
\]

where

\[
\psi_{\text{var}}^s(\rho, \phi) = \frac{2}{\sqrt{s!\pi\sigma_\rho}} \left(\frac{2\rho}{\sigma_\rho}\right)^s e^{-2\rho^2/\sigma_\rho^2 + is\phi} \tag{2.22}
\]

\[
\psi_{\text{var}}(z) = \sqrt{\frac{2}{\pi^{1/2}\sigma_z}} e^{-2z^2/\sigma_z^2}. \tag{2.23}
\]
Here $s$ is the amount of circulation carried by each particle in units of $\hbar$ along the $z$-axis.

### 2.4.2 Variational Energy

Evaluating the total energy, using the variational form Eq. (2.21) in Eq. (2.12) for $s = 0$ and $s = 1$ gives

\[
E_s=0 = \frac{\hbar^2}{M} \left( \frac{2\sigma_z^2 + \sigma_\rho^2}{\sigma_\rho^2 \sigma_z^2} \right) + M \left( \frac{2\omega_\rho^2 \sigma_\rho^2 + \omega_z^2 \sigma_z^2}{16} \right) + \frac{1}{2N} g_s \frac{N g_s}{\pi^{3/2} \sigma_\rho^2 \sigma_z^2} \tag{2.24}
\]

\[
E_s=1 = \frac{\hbar^2}{M} \left( \frac{4\sigma_z^2 + \sigma_\rho^2}{\sigma_\rho^2 \sigma_z^2} \right) + M \left( \frac{4\omega_\rho^2 \sigma_\rho^2 + \omega_z^2 \sigma_z^2}{16} \right) + \frac{1}{2N} g_{dd} \frac{N g_{dd}}{21/2 \pi^{3/2} \sigma_\rho^2 \sigma_z^2} \tag{2.25}
\]

where $f = f \left( \frac{\sigma_\rho}{\sigma_z} \right)$ is given in [51] with the form

\[
f(x) = 1 + 2 \frac{x^2}{1 - x^2} - 3 \frac{x^2 \arctan \left( \sqrt{1 - x^2} \right)}{(1 - x^2)^{3/2}}. \tag{2.26}
\]

Since the DDI energy is proportional to $-f$ [see Eqs. (2.24) and (2.25)]. We can see that for a prolate system, the DDI energy is negative, while for an oblate system, the DDI energy will be positive, from Fig. 2.3.

We give each component of energy (i.e. $E_K$, $E_V$, $E_C$, $E_D$ and $E_{QF}$) in Eqs. (2.24) and (2.25), both of them following the same order as used in Eq. (2.12).

### 2.5 Bogoliubov-de Gennes Equation

To estimate stability of this system we are interested in the collective excitations of the condensate which are Bogoliubov quasiparticles. In order to describe these we linearize the GPE about $\Psi_c$ with a fluctuation field $\vartheta(\mathbf{x}, t)$ as

\[
\Psi(\mathbf{x}, t) = e^{i(S(\mathbf{x}) - \mu t/\hbar)} \left[ \psi(\mathbf{x}) + \vartheta(\mathbf{x}, t) \right] \tag{2.27}
\]

\[
\vartheta(\mathbf{x}, t) \equiv \sum_\nu \left( c_\nu u_\nu e^{-i\epsilon_\nu t/\hbar} - c_\nu^* v_\nu e^{i\epsilon_\nu t/\hbar} \right), \tag{2.28}
\]

where $c_\nu$ is the amplitude of the perturbation, and $u_\nu$ and $v_\nu$ are the particle and hole quasiparticle amplitudes with respective energy $\epsilon_\nu$. We have written the solution of
Figure 2.5: (a) The function $f(x)$ [see Eq. (2.26)] with the colour varying with aspect ratio from prolate (red) to oblate (blue) and the pink cross indicating the zero of $f$ at $x = 1$. Also, $f$ has asymptotic values 1 and $-2$, for the extremely elongated and flattened cases, respectively. (b) and (c) Illustrations of the density isosurface for the cases circled in (a).
the GPE Eq. (2.8), $\Psi_c(x)$ in the form

$$\Psi_c(x) = e^{iS(x)}\psi(x), \quad (2.29)$$

where $\psi(x)$ and the phase $S(x)$ are real. According to time dependent Gross-Pitaevskii equation we have

$$i\hbar \dot{\Psi}(x, t) = \hat{L}\Psi(x, t), \quad (2.30)$$

where

$$\hat{L}f(x, t) \equiv \left[ -\frac{\hbar^2}{2M} \nabla^2 + V_{tr} + \int dx'U(x - x')|f(x', t)|^2 + \gamma_{QF}|f(x, t)|^3 \right] f(x, t). \quad (2.31)$$

and the LHS of Eq. (2.30) applied to Eq. (2.27) gives

$$i\hbar \dot{\Psi}(x, t) = e^{i[S(x) - \mu t/\hbar]} \left\{ \mu \psi(x) + \sum_\nu \left[ (\epsilon_\nu + \mu) c_\nu \bar{v}_\nu e^{-i\bar{\epsilon}_\nu t/\hbar} + (\epsilon_\nu^* - \mu) c_\nu^* v_\nu e^{i\epsilon_\nu t/\hbar} \right] \right\}. \quad (2.32)$$

Note the difference between operators $\hat{L}_{GP}$ and $\hat{L}$: the former is linear in $f$, but the later is non-linear in $f$. When we calculate the RHS of Eq. (2.30) we will only keep terms up to linear order in $\vartheta$. For this we will need

$$|\Psi(x, t)|^3 \approx \psi^3(x) \left\{ 1 + [\vartheta^*(x, t) + \vartheta(x, t)] / \psi(x) \right\}^{3/2} \quad (2.33)$$

$$\approx \psi^3(x) + \frac{3}{2} \psi^2(x) [\vartheta^*(x, t) + \vartheta(x, t)], \quad (2.34)$$

and

$$\int dx'U(x - x')|\Psi(x', t)|^2 \approx g_s \psi(x) [\psi(x) + \vartheta^*(x, t) + \vartheta(x, t)]$$

$$+ \int dx'U_{dd}(x - x')\psi(x') [\psi(x') + \vartheta^*(x', t) + \vartheta(x', t)]. \quad (2.35)$$

Defining

$$\hat{L}_{GP} = e^{-iS(x)}\hat{L}_{GP} e^{iS(x)}, \quad (2.36)$$

we find

$$e^{-i[S(x) - \mu t/\hbar]} \hat{L}\Psi(x, t) \approx \hat{L}_{GP}\psi(x) + \hat{L}_{GP}\vartheta(x, t) + X \left[ \vartheta^*(x, t) + \vartheta(x, t) \right], \quad (2.37)$$
where $X$ is the exchange operator, defined as

$$X f(x) \equiv \psi(x) \int dx' U(x-x') \psi(x') f(x') + \frac{3}{2} \gamma_{QF} |\psi(x)|^3 f(x). \tag{2.38}$$

Using the time independent GPE Eq. (2.8), we have $e^{i\mu t/\hbar} \hat{\Psi}(x, t) - \mu \psi(x) = e^{i\mu t} \hat{L} \hat{\Psi}(x, t) - \hat{L}_{GP} \psi(x)$, so

$$e^{-i[S(x)-\mu t]/\hbar} \hat{\Psi}(x, t) - \mu \psi(x) = e^{-i[S(x)-\mu t]} \hat{L} \hat{\Psi}(x, t) - \hat{L}_{GP} \psi(x). \tag{2.39}$$

We then have

$$\sum_{\nu} \left[ (\epsilon_{\nu} + \mu) c_{\nu} u_{\nu} e^{-i\epsilon_{\nu} t/\hbar} + (\epsilon_{\nu}^* - \mu) c_{\nu}^* v_{\nu}^* e^{i\epsilon_{\nu}^* t/\hbar} \right]$$

$$\approx \hat{L}_{GP} \sum_{\nu} \left( c_{\nu} u_{\nu} e^{-i\epsilon_{\nu} t/\hbar} - c_{\nu}^* v_{\nu}^* e^{i\epsilon_{\nu}^* t/\hbar} \right) + X \sum_{\nu} \left[ c_{\nu}^*(u_{\nu} - v_{\nu}) e^{i\epsilon_{\nu}^* t/\hbar} + c_{\nu}(u_{\nu} - v_{\nu}) e^{-i\epsilon_{\nu} t/\hbar} \right]. \tag{2.40}$$

To ensure this equation holds for all $t$, we find the equations for the coefficients of each term $e^{-i\epsilon_{\nu} t/\hbar}$ and $e^{i\epsilon_{\nu}^* t/\hbar}$, giving two sets of equations

$$(\epsilon_{\nu} + \mu) u_{\nu} = (\hat{L}_{GP} + X) u_{\nu} - X v_{\nu} \tag{2.41}$$

$$(\epsilon_{\nu}^* - \mu) v_{\nu}^* = - (\hat{L}_{GP} + X) v_{\nu}^* + X u_{\nu}^*. \tag{2.42}$$

Since $\mu$ is real and $X$ is hermitian and real, we can write the equations in a general eigenvalue form

$$\begin{pmatrix} \hat{L}_{GP} - \mu + X & -X \\ X & - (\hat{L}_{GP}^* - \mu + X) \end{pmatrix} \begin{pmatrix} u_{\nu} \\ v_{\nu} \end{pmatrix} = \epsilon_{\nu} \begin{pmatrix} u_{\nu} \\ v_{\nu} \end{pmatrix}. \tag{2.43}$$

In the next chapter, we will show how to deal with the operators in Eq. (2.43) by exploiting the symmetry of the system.
Chapter 3
Numerical Methods

The full 3D calculations of the nonlinear stationary states and excitations written in Ch. 2 are numerically expensive to solve. This chapter outlines an efficient and accurate method to solve these problems.

3.1 Numerical Framework

Here we state the algorithms and formalism in a form suitable to perform the numerical calculation. In particular, because we assume cylindrical symmetry, we first adopt the equations presented in the previous chapter to this case.

3.1.1 Gross-Pitaevskii Equation

General Formulation

Several works [57, 29, 31, 37, 32, 33, 36, 30, 58–62] have established that the ground states and dynamics of a dipolar condensate in the droplet regime is well-described by a generalized nonlocal Gross-Pitaevskii equation (GPE). The time-independent stationary state wavefunction $\Psi_c$ is a solution of $\mu \Psi_c = \hat{L}_{GP} \Psi_c$ Eq. (2.8) where

$$\hat{L}_{GP} \equiv -\frac{\hbar^2 \nabla^2}{2M} + V_{tr} + g_s |\Psi_c|^2 + \Phi_{dd}(x) + \gamma_{QF} |\Psi_c|^3,$$

(3.1)

and DDI potential is

$$\Phi_{dd}(x) = \int d \mathbf{x}' U_{dd}(\mathbf{x} - \mathbf{x}') |\Psi_c(\mathbf{x}')|^2.$$

(3.2)

This describes the effects of the long-ranged DDIs, where $U_{dd}(r)$ is from Eq. (2.5). The DDI term here is for the case of dipoles polarized along the $z$ axis by an external field, and $\theta$ is the angle between $r$ and the $z$ axis. The leading-order LHY correction to the chemical potential is included in Eq. (2.20) using the local density approximation.
Cylindrical Formulation

We restrict our attention to a cylindrically symmetric trapping potential, so that the Eq. (2.11) reduces to:

\[ V_{tr}(\rho, z) = \frac{1}{2}M\omega_\rho^2(\rho^2 + \lambda^2 z^2), \quad (3.3) \]

where \( \rho = \sqrt{x^2 + y^2} \), \( \lambda = \omega_z/\omega_\rho \) is the trap aspect ratio, and \( \{\omega_\rho, \omega_z\} \) are the trap frequencies. For this case the entire system is cylindrically symmetric (since we have also chosen the dipoles to be along \( z \)) and we can write 3D stationary solutions Eq. (2.29) in the form

\[ \Psi_c(x) = \psi(\rho, z)e^{is\phi}, \quad (3.4) \]

where \( \phi = \arctan(y/x) \) and \( s \) is an integer specifying the circulation of the vortex. By separating variables in Eqs. (2.8) and (2.36) we arrive at the effective cylindrical GPE

\[ \mu \psi = \mathcal{L}_s \psi, \quad (3.5) \]

\[ \mathcal{L}_s \equiv -\frac{\hbar^2}{2M} \left( D_s + \frac{\partial^2}{\partial z^2} \right) V_{tr} + g_s |\psi|^2 + \Phi_{dd} + \gamma_{QF} |\psi|^3, \quad (3.6) \]

with

\[ D_s \equiv \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} - \frac{s^2}{\rho^2}, \quad (3.7) \]

being the Bessel differential operator. The convolution used to evaluate \( \Phi_{dd} \) Eq. (3.2) is performed in three-dimensions, but the resulting \( \Phi_{dd} \) is a cylindrically symmetric function:

\[ \Phi_{dd}(\rho, z) \equiv \int dx' U_{dd}(x - x')|\psi(\rho', z')|^2, \quad (3.8) \]

\[ = \int \frac{dk_\rho dk_z e^{ik_z z}}{(2\pi)^2} J_0(k_\rho \rho) \tilde{U}_{dd}(k_\rho, k_z) \tilde{n}(k_\rho, k_z), \quad (3.9) \]

where the Fourier transformed density and DDI are

\[ \tilde{n}(k_\rho, k_z) = 2\pi \int d\rho dz \rho J_0(k_\rho \rho)e^{-ik_z z}|\psi(\rho, z)|^2, \quad (3.10) \]

\[ \tilde{U}_{dd}(k_\rho, k_z) = g_{dd} \left( 3 - \frac{k_z^2}{k_\rho^2 + k_z^2} - 1 \right), \quad (3.11) \]

respectively.
We note that here the condensate is normalized to the number of atoms $N$, i.e.

$$2\pi \int_0^\infty d\rho \int_{-\infty}^\infty dz |\psi|^2 = N. \quad (3.12)$$

### 3.1.2 Bogoliubov Excitations

#### Restating the General Formulation

The collective excitations of this system are Bogoliubov quasiparticles, which can be obtained by linearizing the time-dependent GPE Eq. (2.30) about the stationary state as Eq. (2.27). Here we choose the phase in Eq. (2.27) being $S(x) = s\phi$, then we can write the linearized time-dependent GPE in the form

$$\Psi = e^{i(s\phi - \mu t/\hbar)} \left[ \psi + \sum_\nu \left( c_\nu u_\nu e^{-i\epsilon_\nu t/\hbar} - c_\nu^* v_\nu e^{i\epsilon_\nu^* t/\hbar} \right) \right], \quad (3.13)$$

(e.g. see [63, 64]). The Bogoliubov spinor $(u_\nu, v_\nu)$ satisfies the Bogoliubov-de Gennes (BdG) equations Eq. (2.43), and using the defined phase $S(x)$ with Eq. (2.36). The BdG equations are now written in the form

$$\begin{pmatrix} e^{-is\phi} \hat{L}_{\text{GP}} e^{is\phi} - \mu + X & -X \\ -X & -e^{is\phi} \hat{L}_{\text{GP}} e^{-is\phi} - \mu + X \end{pmatrix} \begin{pmatrix} u_\nu \\ v_\nu \end{pmatrix} = \epsilon_\nu \begin{pmatrix} u_\nu \\ v_\nu \end{pmatrix}, \quad (3.14)$$

where the exchange operator $X$ Eq. (2.38) is now in the form

$$X f \equiv \psi \int dx' U(x-x') f(x') \psi(\rho', z') + \frac{3}{2} \gamma_{QF} |\psi|^3 f. \quad (3.15)$$

#### Excitation Properties

Solutions of the BdG equations satisfy the orthogonality condition (e.g. see [65])

$$(\epsilon_\nu - \epsilon_\nu') \int d\mathbf{x} (u_\nu^* u_\nu' - v_\nu^* v_\nu') = 0. \quad (3.16)$$

Setting $\nu = \nu'$ yields $\text{Im}[\epsilon_\nu] \mathcal{N}_\nu = 0$, where

$$\mathcal{N}_\nu = \int d\mathbf{x} (|u_\nu|^2 - |v_\nu|^2), \quad (3.17)$$

is the quasiparticle normalization constant. Thus a solution with a complex energy $\epsilon_\nu$ must have zero-norm, i.e. $\mathcal{N}_\nu = 0$. Such complex energy solutions will exponentially grow with time [see Eq. (3.13)], and indicates that the condensate is dynamically unstable. On the other hand normalizable solutions with $\mathcal{N}_\nu \neq 0$ must have real energies, and we follow convention to scale these solutions so that $\mathcal{N}_\nu = \pm 1$. 


The BdG equations have particle-hole symmetry where given one solution \( \{(u_\nu, v_\nu), \epsilon_\nu\} \), there is a second solution \( \{(u_\nu', v_\nu'), \epsilon_\nu'\} \) obtained by the simple transformation: \( u_\nu' = v_\nu, \quad v_\nu' = u_\nu, \) and \( \epsilon_\nu' = -\epsilon_\nu, \) with \( N_\nu' = -N_\nu \). For a dynamically stable condensate it is conventional to only accept excitations with positive normalization as physical excitations.

We note that there always exists a trivial zero-norm solution that is proportional to the condensate mode, i.e. \( u_0 = \psi, \quad v_0 = \psi \) with \( \epsilon_0 = 0 \). While this solution satisfies the BdG equations written in position space, it can be argued that this mode should be neglected since excitations must be orthogonal to the condensate \[63\].

### Cylindrical Formulation

Utilizing the symmetry of the problem, we can choose the quasi-particle amplitudes to be of the form

\[
 u_\nu = u_{mj}(\rho, z) e^{im\phi}, \quad v_\nu = v_{mj}(\rho, z) e^{im\phi}. \tag{3.18}
\]

The cylindrically symmetric amplitudes \( \{u_{mj}, v_{mj}\} \) satisfy the BdG equations

\[
 \mathcal{M} \begin{pmatrix} u_{mj} \\ v_{mj} \end{pmatrix} = \epsilon_{mj} \begin{pmatrix} u_{mj} \\ v_{mj} \end{pmatrix}, \tag{3.19}
\]

where

\[
 \mathcal{M} = \begin{pmatrix} \mathcal{L}_{m+s} + X_m - \mu & -X_m \\ X_m & -(\mathcal{L}_{m-s} + X_m - \mu) \end{pmatrix}, \quad (3.20)
\]

\[
 X_m f = \psi e^{-im\phi} \int d\mathbf{x}' U_{dd}(\mathbf{x}-\mathbf{x}') e^{im\phi'} f(\rho', z') \psi(\rho', z') + g_s \psi^2 f + \frac{3}{2} |\gamma_F \psi|^3 f. \tag{3.21}
\]

As is apparent by inspection from the expansion Eq. (3.13), the excitations described by \( u_{mj} \) and \( v_{mj} \) have a total \( z \)-component of angular momentum of \( m + s \) and \( m - s \) respectively, so that \( \mathcal{L}_{m+s} \) and \( \mathcal{L}_{m-s} \) operators appear in Eq. (3.20). Note, although not immediately apparent from its form, the DDI part of the exchange operator \( X_m \) is cylindrically symmetric [c.f. Eq. (3.8)].

It is convenient to write Eq. (3.19) as

\[
 \mathcal{M} w_{mj} = \epsilon_{mj} w_{mj}, \tag{3.22}
\]

where we have introduced \( w_{mj} = (u_{mj}, v_{mj})^T \).

We note that given the definition of \( \{u_{mj}, v_{mj}\} \) Eq. (3.18) the particle-hole symmetry relates a solution in the \( m \) angular momentum space to a corresponding negative energy solution in the \( -m \) angular momentum space.
It is also useful to note several exact solutions of the BdG equations. First the trivial zero-norm solution in the \( m = 0 \) subspace \( \{(u_{00}, v_{00}), \epsilon_{00}\} = \{(\psi, \psi), 0\} \). Second, when the system is confined in a harmonic trap there are three Kohn modes [66], which correspond to centre of mass oscillations oscillations along each trap axis occurring at the respective trap frequency. Here we consider a cylindrically symmetric trap and these excitations have energy \( \hbar \omega_z \) in the \( m = 0 \) subspace and \( \hbar \omega_\rho \) in the \( m = \pm 1 \) subspaces. Ensuring these energies are accurately computed is a good check of numerics.

3.2 Numerical Methods for the GPE

3.2.1 Dimensionless Form of the GPE

It is convenient to adopt dimensionless units of length \( x_0 = \sqrt{\hbar/m\omega_0} \) or frequency \( \omega_0 \), and energy \( E_0 = \hbar \omega_0 \) to write the cylindrical GP operator Eq. (3.6) as

\[
\mathcal{L}_s = h + C + D + Q, \tag{3.23}
\]

where we have separated out the key terms for convenience:

\[
h = -\frac{1}{2} \left( D_s + \frac{\partial^2}{\partial z^2} \right) + \frac{1}{2} (\tilde{\omega}_\rho^2 \rho^2 + \tilde{\omega}_z^2 z^2), \tag{3.24}
\]

\[
C = g_s |\psi|^2, \tag{3.25}
\]

\[
D = \int \frac{dk_\rho dk_z}{(2\pi)^2} e^{ik_\rho \rho} J_0(k_\rho \rho) \tilde{U}_{dd}(k_\rho, k_z) \tilde{n}(k_\rho, k_z), \tag{3.26}
\]

\[
Q = \gamma_{QF} |\psi|^3, \tag{3.27}
\]

where we set \( \tilde{\omega}_j = \omega_j / \omega_0 \), \( g_s = 4\pi a_s / x_0 \), \( g_{dd} = 4\pi a_{dd} / x_0 \) [inside \( \tilde{U}_{dd}, \) see Eq. (3.11)] and

\[
\gamma_{QF} = \frac{8}{3\pi^2} g_s \sqrt{\frac{1}{2} g_s^2 (1 + \frac{3}{2} \epsilon_{dd}^2)}, \tag{3.28}
\]

to be the dimensionless interaction parameters, and take all variables to now be dimensionless.

To accurately treat the terms appearing in the GP operator requires a different discretization for the radial and axis dimensions, and we discuss these separately in the next subsections.
3.2.2 Radial Treatment

Bessel Grid and Quadrature

In the radial direction we consider a Bessel grid of $N_\rho$ points that non-uniformly spans the interval $(0, \rho_{\text{max}})$ given by
\[ \rho_{(q)i} = \alpha_{(q)i} \frac{\rho_{\text{max}}}{\alpha_{(q)N_\rho+1}}, \quad i = 1, \ldots, N_\rho. \] (3.29)

Here $\{\alpha_{(q)i}\}$ are the ordered non-zero roots of the Bessel function $J_q(x)$ [see Fig. 3.1] of integer order $q$, which we refer to as the $q$-order Bessel grid. We emphasize that these grid points are not uniformly spaced, see Fig. 3.2. In this work we will have cause to need several such radial grids, each with the same number of points and range but of different orders. For this reason we need to adopt a more cumbersome notation that explicitly indicates order of the Bessel grid. We also introduce the reciprocal space grid of the same order
\[ k_{(q)i} = \alpha_{(q)i} \frac{k_{\text{max}}(q)}{\alpha_{(q)N_\rho+1}} \quad i = 1, \ldots, N_\rho. \] (3.30)

that spans the interval $(0, k_{\text{max}}(q))$, with $k_{\text{max}}(q) = \alpha_{(q)N_\rho+1}/\rho_{\text{max}}$.

These points can be associated with a quadrature-like integration formula [67]
\[ I[g(\rho)] = \int_0^\infty d\rho \rho g(\rho) \approx \sum_{i=1}^{N_\rho} w_{(q)i} g_{(q)i}, \] (3.31)
where $w_{(q)i}$ are the real-space quadrature weights
\[ w_{(q)i} = \frac{2}{(k_{\text{max}}(q))^2 |J_{q+1}(\alpha_{(q)i})|^2}. \] (3.32)

and we have used the notation $g_{(q)i} = g(\rho_{(q)i})$ to denote the function $g(\rho)$ sampled on the $q$-order grid. This integration requires that the functions of interest have limited spatial range, i.e. $g(\rho > \rho_{\text{max}}) = 0$.

Similarly, for $k_\rho$-space we have a quadrature-like integration formula for a function $\tilde{g}(k_\rho)$
\[ I[\tilde{g}(k_\rho)] = \int_0^\infty dk_\rho k_\rho \tilde{g}(k_\rho) \approx \sum_{i=1}^{N_\rho} \tilde{w}_{(q)i} \tilde{g}_{(q)i}, \] (3.33)

and we have used the notation $\tilde{g}_{(q)i} = \tilde{g}(k_{(q)i})$. This integration requires that the functions of interest have limited reciprocal space range, i.e. $\tilde{g}(k_\rho > k_{\text{max}}) = 0$. 

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Figure 3.1: Showing the first four orders of the Bessel function $J_q(x)$. The circles indicate roots for each order of the Bessel function.

Figure 3.2: The spacing of Bessel roots, where $i$ labels the roots $\alpha_{(q)i}$ in ascending order. Note the spacing converges towards $\pi$ as $i \to \infty$. 
where $\tilde{w}_{(q)i}$ are the $k_\rho$-space quadrature weights

$$
\tilde{w}_{(q)i} = \frac{2}{(\rho_{\text{max}}^q)^2 |J_{q+1}(\alpha_{(q)i})|^2},
$$

(3.34)

and $\tilde{g}_{(q)i} = \tilde{g}(k_{(q)i})$. Result Eq. (3.33) is only valid on our grid if the function is bandwidth limited, i.e. $\tilde{g}(k_\rho > k_{(q)i}^\text{max}) = 0$.

**Hankel Transformation**

The Bessel grid is useful because it allows an accurate 2D Fourier transformation of functions of the form $F(\rho) = f^{[q]}(\rho)e^{iq\phi}$, where we have used $\rho$ to denote the planar position vector and the superscript $[q]$ to denote the angular circulation associated with the function. The 2D Fourier transform of $F$ is

$$
\tilde{F}(k_\rho) = \int d\rho e^{-i k_\rho \cdot \rho} F(\rho) = 2\pi i^{-q} e^{iq\phi} \tilde{f}^{[q]}(k_\rho),
$$

(3.35)

where

$$
\tilde{f}^{[q]}(k_\rho) = \int_0^\infty d\rho \rho J_q(k_\rho \rho) f^{[q]}(\rho),
$$

(3.36)

is the $q$-order Hankel transform, arising because the angular integral leads to the appearance of the $J_q$ Bessel function. Here we have introduced $k_\rho$ to represent the 2D $k$-space vector, with polar coordinates $(k_\rho, \phi_k)$. A discrete Hankel transform can be used to obtain $\tilde{f}^{[q]}$ sampled on the $k_{(q)i}$ grid from $f^{[q]}$ sampled on the $\rho_{(q)i}$ grid (see [68]). The explicit form of this discrete transform is obtained by evaluating Eq. (3.36) using the quadrature formula Eq. (3.31)

$$
\tilde{f}^{[q]}_{(q)i} = \mathcal{H}_{ij}^{(q)} f^{[q]}_{(q)j}
$$

(3.37)

(repeated indices summed over) where

$$
\mathcal{H}_{ij}^{(q)} = \frac{2J_q \left( \frac{\alpha_{(q)i} \alpha_{(q)j}}{\alpha_{(q)(N_q+1)}} \right)}{(k_{(q)i}^\text{max})^2 |J_{q+1}(\alpha_{(q)i})|^2},
$$

(3.38)

is the $q$-order Hankel transformation matrix and $f^{[q]}_{(q)j} = f^{[q]}(\rho_{(q)j})$ etc. Here we have explicitly labeled the order of the transformation on $\mathcal{H}$ to emphasize the order of the Bessel functions, and roots appearing in Eq. (3.38). Similarly, the inverse 2D transform

$$
F(\rho) = \int dk_\rho e^{i k_\rho \cdot \rho} \tilde{F}(k_\rho) = \frac{i^{-q} e^{iq\phi}}{2\pi} J_q(k_\rho f^{[q]}(k_\rho),
$$

(3.39)
is accomplished by the inverse Hankel transform

$$f^{[0]}(\rho) = \int_0^\infty dk_\rho k_\rho J_q(k_\rho \rho) \tilde{f}^{[0]}(k_\rho),$$  \hspace{1cm} (3.40)

with discrete form $f_{(q)i}^{[q]} = \mathcal{H}_{ij}^{(q)} \tilde{f}_{(q)j}^{[q]}$, where

$$\mathcal{H}_{ij}^{(q)-1} = \frac{2J_q(a_{(q)j} a_{(q)i})}{(\rho_{\text{max}})^2 |J_{q+1}(a_{(q)j})|^2}.$$  \hspace{1cm} (3.41)

The Discrete Hankel transform is not exactly unitary, but for typical grid sizes ($N_\rho \sim 10^2$) we have that $\mathcal{H}_{ij}^{(q)} \mathcal{H}_{jk}^{(q)-1} \approx \delta_{ij} + O(10^{-9})$, which is adequate for our purposes.

**Interpolation from Bessel Grids**

It is often necessary to be able to interpolate a function on a Bessel grid of a certain order onto a grid of another order, or indeed to some other grid. Given a sampling of the function $f$ on a $q$-Bessel grid $\rho(q)i$, the interpolation on to other points, which we denote as $\bar{\rho}_i$, is accomplished using the linear transformation

$$f(\bar{\rho}_i) = \mathcal{B}_{ij}^{(q)} f_{(q)i},$$  \hspace{1cm} (3.42)

where

$$\mathcal{B}_{ij}^{(q)} = \frac{2\alpha_{(q)j} J_q(k_{\rho_{\text{max}}} \bar{\rho}_i)}{[\alpha_{(q)j}]^2 - (\rho_{\text{max}} \bar{\rho}_i)^2 |J_{q+1}(\alpha_{(q)j})|^2}.$$  \hspace{1cm} (3.43)

The interpolation result we use here was derived in Ref. [69]. In practice we often need to interpolate between Bessel grids of various orders and the relevant matrices $\mathcal{B}$ connecting each grid pair can be generated in advanced and used as needed. For the case which we interpolate to the $q'$-order Bessel grid from a $q$-order Bessel grid (i.e. $\rho(q)i$ to $\rho(q')i$), we denote the associated transform matrix as $\mathcal{B}_{ij}^{(q,q')}$.  

**Radial Laplacian Operator**

Hankel transforms are particularly useful for accurately evaluating the kinetic energy operator in radially symmetric cases (e.g. see [70]). To see this we note that by separating variable the 2D Laplacian $\nabla^2_\rho$ acting on the function $f^{[m]}(\rho)e^{im\phi}$ is equivalent to the Bessel differential operator $D_m$ Eq. (3.7) acting on $f^{[m]}(\rho)$. Using that $J_\nu$ are eigenfunctions of $D_m$, i.e. $D_m J_\nu(k_\rho \rho) = -k_\rho^2 J_\nu(k_\rho \rho)$, we can utilize the Hankel transform
to act on a radial function with $D_m$:

$$D_m f^{[m]} = -\int dk \rho \, k^3 J_q(k \rho) \int \rho' \, J_q(k \rho') f^{[\rho']}(\rho') + \frac{m^2 - q^2}{\rho^2} f^{[m]}(\rho). \quad (3.44)$$

This can be implemented using the $q$-order discrete Hankel transform as

$$D_m f^{[m]}|_{\rho_i} \approx -\mathcal{H}_{ij}^{(q)-1} (k_{(q)j})^2 \mathcal{H}_{jk}^{(q)} f^{[m]}(\rho_k) + \frac{m^2 - q^2}{(\rho_{(q)i})^2} f^{[m]}(\rho_i). \quad (3.45)$$

Clearly it is beneficial to take $m = q$ and avoid the appearance of a centrifugal term, however the freedom to take $m \neq q$ is needed later for our treatment of excitations.

As a example of the Bessel grid, let us consider the dimensionless 2D radially symmetric harmonic oscillator hamiltonian

$$h = -\frac{1}{2} \nabla^2 \rho + \frac{1}{2} \rho^2. \quad (3.46)$$

Eigenstates of $z$-angular momentum $m$ are of the form $\psi_{n_\rho m}(\rho)e^{im\phi}$, with energies

$$\epsilon_{n_\rho m} = 2n_\rho + |m| + 1, \quad (3.47)$$

where $n_\rho = 0, 1, 2, \ldots$ is the radial quantum number. This case can be discretized using a $q$-order Bessel grid as $h_{ij}^{(q)} = T_{ij}^{(q)} + V_{ij}^{(q)}$, where

$$T_{ij}^{(q)} = \frac{1}{2} \mathcal{H}_{ik}^{(q)-1} (k_{(q)j})^2 \mathcal{H}_{kj}^{(q)}, \quad (3.48)$$

is the dense radial kinetic energy operator [see Eq. (3.45)], and

$$V_{ij}^{(q)} = \left[ \frac{q^2 - m^2}{2(\rho_{(q)i})^2} + \frac{1}{2} \frac{1}{(\rho_{(q)i})^2} \right] \delta_{ij}, \quad (3.49)$$

is the diagonal effective potential including the centrifugal term.

Results obtained by diagonalizing $h_{ij}^{(q)}$ are shown in Fig. 3.3. Notably, highly accurate eigenvalues for appropriate choices of Bessel grid order $q$, even for a small number of grid points ($N_\rho = 32$) for even quite high eigenstates [e.g. $n_\rho = 15$ in Fig. 3.3(b)]. In contrast for other choices of $q$ the errors are large. We make the following observations about the choice of Bessel grid order. First, we find that choosing the Bessel grid order $q$ to be the same as $m$ [removing the centrifugal term from Eq. (3.49)] always gives accurate results (red triangles). Second, choosing $q = 0$ for $m$ even or $q = 1$ for $m$ odd (blue circles) also works equivalently well (blue circles). This second observation suggests that the use of two grids ($q = 0, 1$) should suffice for numerical treatment of any $m$ value (also found in [70] [71]).
Figure 3.3: Absolute error in the (a) \( n_\rho = 0 \) and (b) \( n_\rho = 15 \) energy eigenvalues [see Eq. (3.47)] of the radially symmetric harmonic oscillator calculated by diagonalizing the Hamiltonian \( h_{ij}^{(q)} \). The excitation angular momentum \( m \) and the order \( q \) of the Bessel grid used are indicated on the horizontal axis. To aid interpretation results with \( q = m \) are indicated with filled red triangles, cases where \( m \mod 2 = q \) are indicated with blue circles and other cases with crosses. Results calculated using \( N_\rho = 32 \) points with \( \rho^{\text{max}} = 10.5 \).
3.2.3 Axial Treatment

Trigonometric Grids and Quadrature

Our system has reflection symmetry along \( z \) so functions of interest will be of definite parity. We denote such functions as \( f_p(z) \) for even \( p_z = +1 \) or odd \( p_z = -1 \) parity, i.e. \( f_{p_z}(-z) = p_z f_{p_z}(z) \). Due to this symmetry we can use a half-grid on the interval \((0, z_{\text{max}})\) spanned by \( N_z \) equally spaced points

\[
z_j = (j - \frac{1}{2}) \Delta z, \quad j = 1 \ldots N_z, \tag{3.50}
\]

where \( \Delta z = z_{\text{max}} / N_z \). The corresponding reciprocal grid is

\[
k_j = (j - \frac{1}{2}) \Delta k, \quad j = 1 \ldots N_z, \tag{3.51}
\]

where \( \Delta k = \pi / z_{\text{max}} \), which spans the interval \((0, k_{\text{max}})\) with \( k_{\text{max}} = \pi / \Delta z \).

The appropriate quadrature for this grid is the rectangular rule. Only \( p_z = +1 \) functions will have a nontrivial integral given by

\[
I[g^+[z]] = \int_{-\infty}^{\infty} dz \, g^+[z] \approx \sum_{i=1}^{N_z} g_i^+[2\Delta z], \tag{3.52}
\]

where \( g_i^+[z] = g^+[z_i] \). Similarly in \( k_z \)-space we have \( I[\tilde{g}^+[k_z]] = \approx \sum_{i=1}^{N_z} \tilde{g}_i^+[2\Delta k_z] \), where \( \tilde{g}_i^+ = \tilde{g}^+[k_i] \). Here we assume that all real space functions of interest decay to zero by \( z_{\text{max}} \) and \( k \)-space functions decay to zero by \( k_{\text{max}} \).

Cosine and Sine Transformations

The 1D Fourier transform

\[
\tilde{f}^+[k_z] = \int_{-\infty}^{\infty} dz e^{-ik_z z} f^+[z], \tag{3.53}
\]

for functions of definite parity are equivalent to cosine and sine transforms

\[
\begin{align*}
\tilde{f}^+[k_z] &= 2 \int_0^{\infty} dz \cos(k_z z) f^+[z], \tag{3.54} \\
\tilde{f}^-[-k_z] &= 2 \int_0^{\infty} dz \sin(k_z z) f^-[-z]. \tag{3.55}
\end{align*}
\]

Using our assumption that the functions of interest are bandwidth limited in \( z \)- and \( k_z \)-space, we can discretize these transforms on the discrete half grids as

\[
\tilde{f}_i^+ = \Lambda_{ij}^+ f_j^+, \tag{3.56}
\]
where

\[ \Lambda_{ij}^{(p_z)} = \begin{cases} 
2 \cos(k_i z_j) \Delta z, & p_z = +1, \\
2 \sin(k_i z_j) \Delta z, & p_z = -1, 
\end{cases} \]  

(3.57)

are the transformation matrices. These can be identified as the type-IV discrete cosine and sine transformations (e.g. see [72]) and are amenable to fast implementations that avoid the need for carrying out the matrix multiplication indicated in Eq. (3.56).

The inverse Fourier transformation \( f_{\tilde{p}_z}(z) = (2\pi)^{-1} \int_{-\infty}^{\infty} dk_z e^{ik_z z} \tilde{f}_{\tilde{p}_z}(k_z) \) similarly can be mapped to the inverse discrete transform

\[ f_{\tilde{p}_z} = \Lambda_{ij}^{-1(p_z)} \tilde{f}_{\tilde{p}_z}, \]  

(3.58)

where

\[ \Lambda_{ij}^{-1(p_z)} = \begin{cases} 
\frac{1}{2\pi} \cos(k_i z_j) \Delta k, & p_z = +1, \\
\frac{1}{2\pi} \sin(k_i z_j) \Delta k, & p_z = -1, 
\end{cases} \]  

(3.59)

with \( \Lambda_{ij}^{-1(p_z)} \Lambda_{jk}^{(p_z)} = \delta_{ik} \).

**Axial Laplacian Operator**

We can implement a discrete second derivative operator utilizing that the derivative operator is diagonal in \( k_z \)-space, i.e.

\[ \frac{d^2 f_{\tilde{p}_z}}{dz^2} = -\frac{1}{2\pi} \int dk_z k_z^2 e^{ik_z z} \int dz' e^{-ik_z z'} f_{\tilde{p}_z}(z'), \]  

(3.60)

\approx -\Lambda_{ij}^{(p_z)} k_j^2 \Lambda_{jk}^{(p_z)} f_k^{[p_z]}  

(3.61)

As an example of the axial grid, let us consider the dimensionless 1D harmonic oscillator Hamiltonian

\[ h = -\frac{1}{2} \frac{d^2}{dz^2} + \frac{1}{2} z^2. \]  

(3.62)

Eigenstates of parity \( p_z \) have the energies

\[ \epsilon_{n_z p_z} = 2n_z + 1 - \frac{1}{2} p_z, \]  

(3.63)

where \( n_z = 0, 1, 2, \ldots \) is the axial quantum number. This case can be discretized as
\( h_{ij}^{(p_z)} = T_{ij}^{(p_z)} + V_{ij}, \) where
\[
T_{ij}^{(p_z)} = \frac{1}{2} \Lambda_{ij}^{(p_z)} - k_j^2 \Lambda_{jk}^{(p_z)},
\]
is the dense axial kinetic energy operator, and \( V_{ij} = \frac{1}{2} z_i^2 \delta_{ij} \) is the diagonal potential operator (independent of \( p_z \) since both cases have the same grid). Examples of the accuracy of the eigenvalues obtained from the discretized Hamiltonian are shown in Table 3.1. We observe the highly accurate results can be obtained for reasonably high eigenvalues using a modest grid.

<table>
<thead>
<tr>
<th>( n_z )</th>
<th>( p_z = 0 )</th>
<th>( p_z = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( 1.73 \times 10^{-14} )</td>
<td>( 2.07 \times 10^{-14} )</td>
</tr>
<tr>
<td>7</td>
<td>( 2.31 \times 10^{-14} )</td>
<td>( 3.02 \times 10^{-14} )</td>
</tr>
<tr>
<td>15</td>
<td>( 9.13 \times 10^{-09} )</td>
<td>( 4.07 \times 10^{-08} )</td>
</tr>
</tbody>
</table>

Table 3.1: Absolute errors in selected energy eigenvalues of the discrete 1D harmonic oscillator Hamiltonian \( h_{ij} \) computed using \( N_z = 32 \) and \( z^{\max} = 10 \).

### 3.2.4 Cylindrical Treatment

Here we combine the radial and axial treatments to apply to the cylindrical formulations of the GPE. We introduce relevant notations and then focus on how to numerically evaluate key operators needed for them (and later also for the excitations).

The cylindrical functions we introduce will be evaluated on cylindrical (2D) mesh of points consisting of the radial and axial points \((\rho_i, z_j)\) introduced earlier. We shall refer to this as a \( q \)-order cylindrical grid. To properly account for the properties of the functions we are working and the Bessel grid it is discretized on, so we introduce the notation
\[
F(r) = f^{[sp_z]}(\rho, z)e^{is\phi} \rightarrow f^{[sp_z]}_{(q)ij} = f(\rho(q)_{ij}, z_j),
\]
for a function of definite \( z \)-parity of \( p_z \) and angular circulation \( s \) discretized on the \( q \)-order cylindrical grid. While this notation is somewhat cumbersome, we have found it quite important to be clear about the properties of the functions to identify the correct quadratures and transformations to apply on evaluating the required operations numerically. This allows us in general to work simply with the cylindrical fields \( f \) and avoid constructing any 3D fields that would be of significantly higher computational cost.
We note that properties of the cylindrical fields can change with operations. For example, consider a 3D field $G$ given by modulus squared operation $G = |F|^2$, where the field $F$ has unit circulation and odd parity (i.e. $p_z = -1$ and $s = 1$). By inspection we see that $G = g^{[0+]}$, i.e. the new cylindrical field $g^{[0+]} = (f^{[1-]})^2$ has no angular circulation and even-z-parity\footnote{Alternatively, we can exploit our notation more fully and note that because of the conjugation of a field in the density we have $g^{[0+]} = f^{-s-}f^{[s+]}$, with the circulation of $g$ determined by the sum of the circulations of those on the right hand side, and the parity determined by the product of the parities on the right hand side.}

In this section we wish to evaluate the basic numerical operators [as defined in Eq. (3.23)] that will act on the field cylindrical condensate field Eq. (3.4) discretized on a cylindrical grid

$$\psi^{[spz]}(\rho, z) \rightarrow \psi^{[spz]}(q_{ij}),$$ (3.66)

We will generically denote these operators $O$ as

$$O[f^{[spz]}(q))] = \mathcal{O}[f^{[spz]}(q_{ij})],$$ (3.67)

adopting a calligraphic script for the numerical form acting on the discretized function. In general these operators will depend on $q$, $s$ and $p_z$.

We also introduce the quadrature integration for 3D integration in real space

$$I_r[f^{[spz]}(q)] = \sum_{i,j} 4\pi \Delta z \, w(q_{ij}) f^{[s+]}(q_{ij}) \delta_{p_z,0} \delta_{s,0},$$ (3.68)

and $k$-space

$$I_k[f^{[spz]}(q)] = \sum_{i,j} 4\pi \Delta k \, \tilde{w}(q_{ij}) \tilde{f}^{[s+]}(q_{ij}) \delta_{p_z,0} \delta_{s,0}.$$ (3.69)

This quadrature is the immediate generalization of the quadratures introduced in Secs. 3.2.2 and 3.2.3

**Single Particle Operators**

The single particle operator $h$ [see Eq. (3.24)] has both the kinetic and potential parts. It is convenient to divide this operator into two parts. First, a differential part ($T$) involving the Bessel differential operator and axial second derivative. Second, a part ($V$) that is local in position space, and includes the potential and centrifugal terms.

Applying our discretization on the first part $-\frac{1}{2}(D_s + \frac{\partial^2}{\partial z^2})\psi$ we arrive at the

$$T = T_{ik} \psi^{[spz]}(q_{ik}) + \psi^{[spz]}(q_{ik}) T^{(p_z)}_{ik},$$ (3.70)
where $T^{(q)}_{ik}$ and $T^{(p_z)}_{ik}$ are the radial and axial kinetic energy operators introduced earlier.

The second part is local (diagonal) in position space and is discretized as

$$V \left[ \psi_{(q)}^{[sp_z]} \right] = \frac{1}{2} \left( \hat{\omega}^2 (\rho_{(q)ij})^2 + \hat{\omega}^2 \tau^2 \right) \psi_{(q)ij}^{[sp_z]} \left( \frac{s^2 - q^2}{2(\rho_{(q)ij})^2} \right) \psi_{(q)ij}^{[sp_z]} \text{ (no sum)}.$$  \hspace{1cm} (3.71)

Here \text{no sum} indicates that repeated indices are not summed over.

**Local Interaction Terms**

The contact interaction $g_s \psi^3$ is diagonal in position space and given by

$$C \left[ \psi_{(q)}^{[sp_z]} \right] = g_s \left( \psi_{(q)ij}^{[sp_z]} \right)^3 \text{ (no sum)},$$  \hspace{1cm} (3.72)

and similarly for the quantum fluctuation term $\gamma_{QF} |\psi|^3 \psi$

$$Q \left[ \psi_{(q)}^{[sp_z]} \right] = \gamma_{QF} \left( \psi_{(q)ij}^{[sp_z]} \right)^3 \psi_{(q)ij}^{[sp_z]} \text{ (no sum)}.$$  \hspace{1cm} (3.73)

**Fourier Transforms**

The 3D Fourier transform of a function can be evaluated by combining the radial Eq. (3.35) and axial Eq. (3.53) transforms introduced earlier. The discrete Fourier transform is given by

$$\mathcal{F} \left[ f_{(q)}^{[sp_z]} \right] = 2\pi i^{-s} e^{is\phi} B^{(s,q)}_{la} \mathcal{H}^{(s)}_{ab} B^{(q,s)}_{bk} f_{(q)kl}^{[sp_z]} \Lambda_{lj}^{(p_z)}.$$  \hspace{1cm} (3.74)

An important feature to note here is that because the field being transformed has an angular circulation of $s$ the $s$-order Hankel transform needs to be used. For this to be computed accurately we must interpolate the function onto the $s$-order grid (i.e. $B^{(q,s)}$) before performing the Hankel transform, and then subsequently transform back to the desired output grid $q$.

Similarly, the inverse transform is given by

$$\mathcal{F}^{-1} \left[ \tilde{f}_{(q)}^{[sp_z]} \right] = \frac{i^{-s} e^{is\phi}}{2\pi} B^{(s,q)}_{la} \mathcal{H}^{-1(s)}_{ab} B^{(q,s)}_{bk} \tilde{f}_{(q)kl}^{[sp_z]} \Lambda_{lj}^{(p_z)-1}.$$  \hspace{1cm} (3.75)

**DDI Term**

The DDI effective potential can be evaluated using the convolution theorem

$$\Phi_{dd} = \frac{1}{(2\pi)^3} \int d\kappa e^{ikr} \hat{U}_{dd}(\kappa) \hat{n}(\kappa),$$  \hspace{1cm} (3.76)
where \( \hat{n} \) is the Fourier transform of the condensate density \( |\Psi|^2 = |\psi(\rho, z)|^2 \), and

\[
\hat{U}_{dd}(\mathbf{k}) = \hat{U}_{dd}(k_\rho, k_z) = g_{dd} \left( 3 \frac{k_\rho^2}{k_\rho^2 + k_z^2} - 1 \right), \tag{3.77}
\]

is the Fourier transform of \( U_{dd}(\mathbf{r}) \). Here we have used tildes indicate quantities in \( k \)-space. The density is \( n_{(q)}^{(0+)} = \left( \psi_{(q)}^{(spz)} \right)^2 \) and we can use the numerical Fourier transforms [see Sec. 3.2.4] to obtain \( \hat{n}_{(q)}^{(0+)} = \mathcal{F} \left[ n_{(q)}^{(0+)} \right] \), and hence

\[
\Phi_{dd(q)}^{(0+)} = \mathcal{F}^{-1} \left[ \hat{U}_{dd(q)}^{(0+)} \mathcal{F} \left[ \left( \psi_{(q)}^{(spz)} \right)^2 \right] \right]. \tag{3.78}
\]

Here \( \hat{U}_{dd(q)}^{(0+)} \) and \( \Phi_{dd(q)}^{(0+)} \) denotes Eqs. (3.77) and (3.76) sampled on the 0-order \( k \)-space cylindrical grid, respectively. Thus the full DDI term is

\[
\mathcal{D} \left[ \psi_{(q)}^{(spz)} \right] = \Phi_{dd(q)}^{(0+)} \psi_{(q)}^{(spz)}. \tag{3.79}
\]

The analytic form Eq. (3.77) is badly behaved in the sense that the \( k \to 0 \) limit does not exist, reflecting the long-ranged anisotropic character of the interaction. Thus using the bare \( k \)-space DDI is not ideal, and results converge slowly as the grid extent is increased. A simple fix to this problem was first proposed in Ref. [64], in which it was shown the convergent results can be obtained with an adequate grid if a cutoff \( U_{dd} \) potential was introduced. This potential is defined as the normal DDI potential, but is set to zero outside of some range of interest, and then a cutoff \( \hat{U}_{dd} \) is obtained by Fourier transforming this truncated function. Analytic results for the cutoff \( \hat{U}_{dd} \) are only known for simple cutoff shapes. For example, the spherical cutoff interaction \( k \)-space interaction \( \hat{U}_{dd}^{r\text{cut}} \) is defined as the Fourier transform of the truncated real space interaction

\[
U_{dd}^{r\text{cut}}(\mathbf{r}) = \begin{cases} 
3 g_{dd} \frac{1}{4\pi} (1 - 3 \cos^2 \theta), & r \leq r_{\text{cut}} \\
0, & \text{otherwise}
\end{cases}, \tag{3.80}
\]

The analytic result [64] is

\[
\hat{U}_{dd}^{r\text{cut}}(\mathbf{k}) = g_{dd} \left( 1 + 3 \frac{\cos(kr_{\text{cut}})}{(kr_{\text{cut}})^2} - 3 \frac{\sin(kr_{\text{cut}})}{(kr_{\text{cut}})^3} \right) \times \left( \frac{3k^2}{k^2} - 1 \right), \tag{3.81}
\]

with \( k^2 = k_\rho^2 + k_z^2 \).

For the solutions we are interested in, they are localized within the cylindrical region of space \( V_{\text{cyl}} = \{ \rho < \rho_{\text{max}}, |z| < z_{\text{max}} \} \), and a truncated \( k \)-space potential can be
calculated as the Fourier transform of the truncated real-space DDI potential

\[
U_{dd}^{\text{cyl}}(r) = \begin{cases} 
\frac{3g_{dd}}{4\pi r^3}(1 - 3 \cos^2 \theta), & r \in V_{\text{cyl}} \\
0, & \text{otherwise} \end{cases}
\]  

(3.82)

The Fourier transform of this truncated kernel, \( \tilde{U}_{dd}^{\text{cyl}} \), needs to be calculated numerically and is essential for accurate solutions in highly anisotropic geometries we consider \(^2\). For all the results we present we use \( \tilde{U}_{dd}^{\text{cyl}} \) (unless stated otherwise) to evaluate the dipole interaction Eq. (3.79). We refer the interested reader to Ref. [19] for details about the numerical calculation.

### 3.2.5 Gross-Pitaevskii Operator and Energy Functional

We have now discussed all the operators needed to evaluate the GP operator i.e.

\[
\mathcal{L}_s \left[ \psi^{[spz]}(q) \right] = \mathcal{T} \left[ \psi^{[spz]}(q) \right] + \mathcal{V} \left[ \psi^{[spz]}(q) \right] + \mathcal{C} \left[ \psi^{[spz]}(q) \right] + \mathcal{D} \left[ \psi^{[spz]}(q) \right] + \mathcal{Q} \left[ \psi^{[spz]}(q) \right],
\]

(3.83)

The expectation of the GP operator, normalized by the field norm \( N \), gives the expected value of the chemical potential, and corresponds to the GP eigenvalue \( \mu \) for the case of a stationary state of the GP operator. This expectation is evaluated numerically as

\[
\mu_{\text{GP}} \left[ \psi^{[spz]}(q) \right] = \frac{1}{N} I_r \left[ \psi^{[spz]}(q) \mathcal{L}_s \left[ \psi^{[spz]}(q) \right] \right].
\]

(3.84)

We can also construct the energy density

\[
\mathcal{E} \left[ \psi^{[spz]}(q) \right] = \psi^{[spz]}(q) \left( \mathcal{T} \left[ \psi^{[spz]}(q) \right] + \mathcal{V} \left[ \psi^{[spz]}(q) \right] + \frac{1}{2} \mathcal{C} \left[ \psi^{[spz]}(q) \right] + \frac{1}{2} \mathcal{D} \left[ \psi^{[spz]}(q) \right] + \frac{2}{5} \mathcal{Q} \left[ \psi^{[spz]}(q) \right] \right),
\]

(3.85)

and the integral of this gives the total energy of the field \( E \left[ \psi^{[spz]}(q) \right] = I_r \left[ \mathcal{E} \left[ \psi^{[spz]}(q) \right] \right] \).

### 3.2.6 Gaussian Variation Solution

It is useful to have a simple variational solution for making predictions for stationary state solutions and validating the accuracy of our numerical methods. Although we have been already mentioned about it in Sec. 2.4, but in this section we will reiterate about it in a more detail description and involve notations which has been introduced

\(^2\)We emphasize because of the singular nature of the potential, it is not adequate to use the Fourier transform introduced in Sec. 3.2.4 and a special treatment of this integral is required.
Here we consider a gaussian state with angular circulation of \( s \)

\[
\Psi_G(r) = \psi_G^{[s+]}(\rho, \sigma) e^{i \phi},
\]

(3.86)

where the cylindrical amplitude \( \psi_G^{[s+]} \) is the same as Eq. (2.21) and the widths \( \{ \sigma_\rho, \sigma_z \} \) are considered as variational parameters.

We can use this state to separately evaluate the energy terms analytically using Eq. (2.12) or the operators defined in Eq. (3.23), i.e. defining

\[
E_h = \langle h \rangle,
\]

\[
E_C = \langle \frac{1}{2} C \rangle,
\]

\[
E_D = \langle \frac{1}{2} D \rangle,
\]

\[
E_Q = \langle \frac{2}{5} Q \rangle,
\]

where \( \langle h \rangle = \int dr \psi_G^{[s+]} h \psi_G^{[s+]} \), \( \langle \frac{1}{2} C \rangle = \int dr \frac{1}{2} g_s (\psi_G^{[s+]})^4 \), etc.

Evaluating these integrals we obtain

\[
E_h = N \left( \frac{2 + 2s}{\sigma_\rho^2} + \frac{1}{\sigma_z^2} + \frac{1 + s}{8} \omega_\rho^2 \sigma_\rho^2 + \omega_z^2 \sigma_z^2 \right),
\]

(3.87)

\[
E_C = N^2 \left( \frac{2}{\pi} \right)^{\frac{3}{2}} \frac{g_s}{2 \sigma_\rho^2 \sigma_z},
\]

(3.88)

\[
E_D = - N^2 \left( \frac{2}{\pi} \right)^{\frac{3}{2}} \frac{(2s!)}{4^{s}(s!)^2} 2\sigma_\rho^2 \sigma_z \sum_{n=0}^{2s+1} d_n^{(s)} f(n) \left( \frac{\sigma_z}{\sigma_\rho} \right),
\]

(3.89)

\[
E_Q = N^2 \frac{2^{7+5s/2} \Gamma(1 + 5s/2)}{(5^{1+s}s!)^{5/2} \pi^{9/4} \sigma_\rho^3 \sigma_z^{3/2}},
\]

(3.90)

where \( f(x) \) is in Eq. (2.26), and for \( s = 0, 1, 2 \)

\[
d_n^{(s)} = \begin{cases} 
1, & s = 0, \\
1 + \frac{s}{4}, & s = 1, \\
1 + \frac{67}{128}, & s = 2.
\end{cases}
\]

(3.91)

By summing Eqs. (3.92)-(3.95) for the case of \( s = 0 \) and \( s = 1 \), and divide by number of atoms \( N \). We will again retrieve Eqs. (2.24) and (2.25), respectively.

### 3.2.7 Variational Solution Test of the Numerical Algorithm

We use these analytic results Eqs. (3.87)-(3.90) to benchmark the accuracy of our numerical evaluation of the various terms appearing in the GPE. To do this we can sample the variational gaussian solution of a \( q \)-order cylindrical grid [i.e. \( \psi_G^{[s+]_{ij}} \)], and
then numerically evaluate the terms corresponding to the energy contributions, i.e.

\[ E_{\text{num}}^h = I_r \left[ \psi_{G(q)}^{[s]} \left( T \left[ \psi_{G(q)}^{[sp]} \right] + V \left[ \psi_{G(q)}^{[sp]} \right] \right) \right], \]  

(3.92)

\[ E_{\text{num}}^C = I_r \left[ \psi_{G(q)}^{[s]} \frac{1}{2} C \left[ \psi_{G(q)}^{[s]} \right] \right], \]  

(3.93)

\[ E_{\text{num}}^D = I_r \left[ \psi_{G(q)}^{[s]} \frac{1}{2} D \left[ \psi_{G(q)}^{[s]} \right] \right], \]  

(3.94)

\[ E_{\text{num}}^Q = I_r \left[ \psi_{G(q)}^{[s]} \frac{2}{5} Q \left[ \psi_{G(q)}^{[s]} \right] \right]. \]  

(3.95)

We compare the numerical and exact results in Table 3.2. We make a few observations. First, as noted in our test of the radial grid with the harmonic oscillator Hamiltonian, we can use \( q = 0 \) or \( q = 1 \) for even or odd \( s \), respectively, and obtain accurate evaluation of the kinetic energy (in \( E_h \)). Most other terms are insensitive to the Bessel order of the grid. In general these results show that \( E_D \) is the most challenging energy to calculate accurately.

We present results for three choices of the DDI potential: the bare interaction \( \hat{U}_{dd} \), spherically cutoff (\( \hat{U}_{dd}^{\text{r cut}} \)) and cylindrically cutoff (\( \hat{U}_{dd}^{\text{cyl}} \)) DDI interactions. For the spherically cutoff DDI potential \( \hat{U}_{dd}^{\text{r cut}} \) we take \( r_{\text{cut}} = \max[\rho_{\text{max}}, z_{\text{max}}] \).

<table>
<thead>
<tr>
<th>case</th>
<th>( \psi_{G}^{[s]} ) parameters</th>
<th>cylindrical grid</th>
<th>relative energy error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( (\sigma_\rho, \sigma_z) )</td>
<td>( (N_\rho, N_z) )</td>
<td>( (\rho_{\text{max}}, z_{\text{max}}) )</td>
</tr>
<tr>
<td>a</td>
<td>( (2,1) )</td>
<td>64,64</td>
<td>(8,4)</td>
</tr>
<tr>
<td>b</td>
<td>( (2,1) )</td>
<td>64,128</td>
<td>(8,8)</td>
</tr>
<tr>
<td>c</td>
<td>( (0.5,4) )</td>
<td>64,64</td>
<td>(2,16)</td>
</tr>
<tr>
<td>d</td>
<td>( (2,1) )</td>
<td>64,64</td>
<td>(8,4)</td>
</tr>
<tr>
<td>e</td>
<td>( (2,1) )</td>
<td>64,128</td>
<td>(8,8)</td>
</tr>
<tr>
<td>f</td>
<td>( (0.5,4) )</td>
<td>64,64</td>
<td>(2,16)</td>
</tr>
<tr>
<td>g</td>
<td>( (0.5,4) )</td>
<td>64,64</td>
<td>(2,16)</td>
</tr>
<tr>
<td>h</td>
<td>( (0.5,4) )</td>
<td>64,64</td>
<td>(2,16)</td>
</tr>
<tr>
<td>i</td>
<td>( (0.5,4) )</td>
<td>64,64</td>
<td>(2,16)</td>
</tr>
<tr>
<td>j</td>
<td>( (0.5,4) )</td>
<td>64,64</td>
<td>(2,16)</td>
</tr>
</tbody>
</table>

We compare the numerical and exact results in Table 3.2. We make a few observations. First, as noted in our test of the radial grid with the harmonic oscillator Hamiltonian, we can use \( q = 0 \) or \( q = 1 \) for even or odd \( s \), respectively, and obtain accurate evaluation of the kinetic energy (in \( E_h \)). Most other terms are insensitive to the Bessel order of the grid. In general these results show that \( E_D \) is the most challenging energy to calculate accurately.
the spherically $U_{dd}^{\text{rad}}$ and cylindrically $U_{dd}^{\text{cyl}}$ cutoff interactions [see Sec. 3.2.4]. Evaluating $E_D$ using the bare interaction is always inaccurate, and converges slowly to the exact result as the grid range increases [cf. case (a) and (b)]. The spherically cutoff interaction is useful in cases where the grid has a similar radial and axial range, and is thus efficient for states where the density distribution has a similar radial and axial extent [cf. cases (b) and (e)]. The cylindrically cutoff interactions works well in all cases including highly anisotropic situations.

3.2.8 Solving the GPE

Gradient Flow Solution Technique

Here we present a simple gradient flow solver based on our discretization. This is an energy minimising scheme for finding ground states. The gradient flow involves solving the time-dependent GPE in imaginary time, i.e. solving the flow $\dot{\psi} = -L_s \psi$. However, normalization of the field tends to decrease under this evolution, so it is necessary to renormalize during the evolution. We follow Ref. [73] (also see [74]) and descretize the evolution using a backwards-forwards Euler scheme. Here time is advanced in time steps $\Delta t$ to the times $t_n = n \Delta t$. During such a step the updated wavefunction $\psi^+$ is obtained from the current field $\psi(t_n)$ according to

$$\frac{\psi^+-\psi(t_n)}{\Delta t} = \frac{1}{2} \left( D_s + \frac{\partial^2}{\partial z^2} \right) \psi^+ - V_{\text{eff},n} \psi(t_n) + \alpha[\psi(t_n) - \psi^+], \quad (3.96)$$

$$\psi(t_{n+1}) = \sqrt{\frac{N \psi^+}{\int |\psi^+|^2 dr}}, \quad (3.97)$$

where Eq. (3.97) is the renormalization (projection),

$$V_{\text{eff},n} = \frac{1}{2} (\tilde{\omega}_\rho^2 \rho^2 + \tilde{\omega}_z^2 z^2) + \Phi_{dd} + \gamma_{\text{GF}} |\psi(t_n)|^3 - \mu_{\text{GP}}[\psi(t_n)], \quad (3.98)$$

and the chemical potential expectation cf. Eq. (3.84). By subtracting $\mu_{\text{GP}} \psi(t_n)$ for the evolution equation we ensure that to $O(\Delta t^2)$ the field normalization is constant under the gradient flow (e.g. see [75]). The parameter $\alpha \geq 0$ is a stabilization parameter [see [73]] allowing larger time steps. Here we take $\alpha$ to be

$$\alpha = \frac{1}{2} \left[ \max(V_{\text{eff},n}) + \min(V_{\text{eff},n}) \right], \quad (3.99)$$
with the max and min evaluated on the spatial grid used to discretize $\psi$. When $\alpha \geq 0$, then the optimal bound for the time step is (see Sec. 3.2 of [73])

$$\Delta t < \frac{1}{\alpha}. \quad (3.100)$$

The semi-implicit equation Eq. (3.96) has the formal solution

$$\psi^+ = \frac{[1 + (\alpha - V_{\text{eff},n})\Delta t]\psi(t_n)}{1 - \frac{1}{2} \left(D_s + \frac{\partial^2}{\partial x^2} - 2\alpha\right) \Delta t}, \quad (3.101)$$

which can be evaluated using Fourier transforms

$$\psi^+ = \mathcal{F}^{-1} \left[ \mathcal{F} \left[ 1 + (\alpha - V_{\text{eff},n})\Delta t\psi(t_n) \right] \right] \left[ 1 + \frac{1}{2} \left(k_x^2 + k_y^2 + 2\alpha\right) \Delta t \right]. \quad (3.102)$$

This can be efficiently implemented numerically using the operators and transforms we introduced earlier.

Alternatively the GPE can be solved using a conjugate gradient technique. This technique can be significantly more efficient than the gradient flow method for many applications. However, this technique is detailed in Ref. [75] for rotating condensates (also see [64]) and we do not explain it further here.

**Stationary State Examples**

Here we give two examples of the gradient flow solver applied to a $s = 1$ vortex state. We characterize the quality of the stationary solutions according to the residual

$$\text{resid} = \max \left| \mathcal{L}_s[\psi_{s+}^{(q)}] - \mu_{\text{GP}}[\psi_{s+}^{(q)}] \psi_{s+}^{(q)} \right|,$$  

with the maximum taken over all spatial points of the solution field.

We give an example of the gradient flow solution in Fig. 3.4 for trap-bound [see Fig. 3.4(a)] and self-bound [see Fig. 3.4(b)] vortex states. In both cases we terminate the flow when we obtain a residual of $10^{-8}$, at which point the absolute error in the energy $|E - E_{\text{final}}|$ on the grid used is $\lesssim 10^{-9}$.

For the trap bound state the stabilization parameter is $\alpha = 185$ (evaluated in the final state), suggesting a time step bound of $\Delta t < 0.0054$. We use $\Delta t = 0.006$ for our results, noting that larger time steps also converge, although the number of steps required does not appreciably decrease with larger time steps.

For the self-bound state we require $\Delta t \lesssim 2 \times 10^{-3}$ for the flow to converge. Here $V_{\text{eff},n}$ is everywhere negative as the droplet is self-bound and there is no harmonic trapping. As a result the stabilization parameter $\alpha$ is negative, and cannot be used to improve the stability or provide an estimate of the time step. In this case we adjust
Figure 3.4: Gradient flow evolution for vortex stationary states. The final stationary solutions for \( s = 1 \) vortex states for (a) a trapped case with \((g_s, g_{dd}) = (0.08, 0.08), \tilde{\omega}_\rho = 1\) and \(\tilde{\omega}_z = 5\), and (b) an non-trapped case of a self-bound vortex droplet with \((g_s, g_{dd}) = (0.045, 0.08)\). In both cases we take \(N = 1 \times 10^4\). In (c) and (d) we show the evolution of the residual Eq. (3.103) for cases (a) and (b), using \(\Delta t = 6 \times 10^{-3}\) and \(2 \times 10^{-3}\), respectively. The initial state for both cases is Eq. (2.21) with \((\sigma_\rho, \sigma_z) = (0.5, 4)\). The gradient flow is terminated when the residual gets to \(10^{-8}\). The insets show the evolution of the system energy during the gradient flow, with \(E_{\text{final}}\) being the energy of the final state. State (a) is calculated on a grid \((N_\rho, N_z) = (128, 128)\) with \((\rho^{\text{max}}, z^{\text{max}}) = (5, 14)\), and has \(E/N = 17.017, \mu = 20.978\). State (b) is calculated on a grid \((N_\rho, N_z) = (128, 128)\) with \((\rho^{\text{max}}, z^{\text{max}}) = (3, 14)\), and has \(E/N = 0.42516, \mu = -5.9603\). Note that \(\gamma_{\text{QF}}\) is given by Eq. (3.28).
the time step until we find that the flow converges. On a current generation laptop the two flows require about 5 seconds and 25 seconds, respectively.

### 3.3 Numerical Methods for the BdG Excitations

Equation (3.22) is not directly amenable to standard large-scale eigenvalue techniques. First, while \( L_{m\pm s} \) and \( X_m \) are real symmetric operators (i.e. hermitian), the full BdG matrix \( \mathcal{M} \) is not. Thus complex eigenvalues can occur. Second, the excitation spectrum is unbounded from above and below (i.e. the particle-hole symmetry), while the excitations of interest occur in the middle of the spectrum, typically those excitations with the lowest positive real part of energy.\(^3\)

We employ two different methods for solving the BdG excitations. Common to both approaches is that we use large scale numerical eigenvalue techniques, notably some version Lanczos algorithm, available through ARPACK \([76]\) (e.g. via the EIGS command in Matlab using Krylov-Schur algorithm \([77]\)). These algorithms are useful in that they can find a subset of the spectrum without the full matrix needing to be constructed, i.e. we simply need to be able to apply the operator to arbitrary vectors. This is useful because the matrices of interest are naturally represented on the cylindrical grids with of the order of \( N_{\text{pts}} \sim 10^4 \) to \( 10^5 \) points, and the associated matrices are of size \( \sim N_{\text{pts}} \times N_{\text{pts}} \), (with the BdG matrix being a factor of 2 larger in each dimension). The matrices of interest are dense and for \( N_{\text{pts}} = 10^4 \) \((N_{\text{pts}} = 10^5)\) matrices such as \( L_s \) require approximately 800MB (80GB) of memory storage. The Lanczos type algorithms are very effective at calculating the extremal eigenvalues, such as those with the largest magnitude, or the largest or smallest, real or imaginary part. However, as noted above for the full BdG problem, the eigenstates of interests are in the middle of the spectrum, typically the eigenvalues of the smallest magnitude. Lanczos type algorithms can only compute the smallest magnitude eigenvalues if you can act with the inverse matrix. This is not convenient and we need to explore two alternatives.

First in Sec. 3.3.1 we construct a basis from a related Hermitian problem. The related problem has a real spectrum bounded from below and we can use Lanczos type algorithms by searching for the smallest real eigenvalues (which are the extremal values in this case). Finding a basis of up to \( N_B \sim 10^3 \) vectors, we then project the BdG equations onto this basis to arrive at a matrix small enough to be directly diagonalized using standard numerical methods.

Second, in Sec. 3.3.2, we instead recast the BdG equations by effectively squaring them. This makes the spectrum real and non-negative. Importantly, the smallest

\(^3\)We note that for vortices positively normed Eq. (3.17) excitations can occur with a negative real energy. We also note that complex excitations (dynamic instabilities) are of interest and are unnormalized.
magnitude eigenvalues are now the extremal eigenvalues (i.e. smallest real) and can be calculated using Lanczos type algorithms.

In this section we shall assume that the condensate has even \( z \)-parity for simplicity, i.e. \( \psi^{[s+]} \).

### 3.3.1 Basis Set Solutions

One approach to solving the BdG equations involves making a basis set expansion of the quasiparticles

\[
u_{mj}(\rho, z) = \sum_{k=1}^{N_B} c^j_k \eta^+_k(\rho, z), \tag{3.104}\]
\[
v_{mj}(\rho, z) = \sum_{k=1}^{N_B} d^j_k \eta^-_k(\rho, z), \tag{3.105}\]

where \( \{\eta^+_k\} \) and \( \{\eta^-_k\} \) are each an orthonormal real basis and \( \{c^j_k, d^j_k\} \) are the expansion coefficients of the \( j \)-th eigenstate. Here we have restricted the summation to \( N_B \) basis set elements. We can then project the BdG Eq. (3.19) onto this basis to obtain the eigensystem

\[
\mathcal{M}_B \begin{pmatrix} c^j \\ d^j \end{pmatrix} = \epsilon_{mj} \begin{pmatrix} c^j \\ d^j \end{pmatrix}, \tag{3.106}\]

where we have used \( c^j \) and \( d^j \) to represent the vector of expansion coefficients. Also, \( \mathcal{M}_B \) is the \( 2N_B \times 2N_B \) matrix obtained by projecting \( \mathcal{M} \) onto the basis, which takes the block form

\[
\mathcal{M}_B = \begin{pmatrix} L_{++} + X_{++} - \mu & -X_{+-} \\ X_{-+} & -(L_{--} + X_{--} - \mu) \end{pmatrix}, \tag{3.107}\]

where the \( N_B \times N_B \) submatrices have elements

\[
(L_{++})_{kk'} = 2\pi \int \rho d\rho d\eta \eta^{+}_k \mathcal{L}_{m+s, \eta^{+}_{k'}} , \tag{3.108}\]
\[
(L_{--})_{kk'} = 2\pi \int \rho d\rho d\eta \eta^{-}_k \mathcal{L}_{m-s, \eta^{-}_{k'}} , \tag{3.109}\]
\[
(X_{\theta\varphi})_{kk'} = 2\pi \int \rho d\rho d\eta \eta^{\theta}_k \mathcal{L}_{m, \eta^{\varphi}_{k'}} , \quad \theta, \varphi \in \{+, -\}. \tag{3.110}\]

In the following subsections we explore two choices of basis functions for this expansion.
Hartree Basis Method

The Hartree basis sets are defined as the normalized eigenstates

\[
\mathcal{L}_{m+s} \eta_k^+(\rho, z) = E_k^+ \eta_k^+(\rho, z),
\]

(3.111)

\[
\mathcal{L}_{m-s} \eta_k^-(\rho, z) = E_k^- \eta_k^-(\rho, z),
\]

(3.112)

where \( E_k^+ \) and \( E_k^- \) are the Hartree energies. These modes are also referred to as the GP basis as they form a set of orthogonal modes to the GPE stationary state. In this basis the \( L_{\pm \pm} \) matrices are diagonal, but it remains to compute the exchange operator matrix elements [see Sec. 3.3.1].

Hartree-Fock Basis Method

The Hartree-Fock basis sets sets are defined as the normalized eigenstates

\[
(\mathcal{L}_{m+s} + X_m) \eta_k^+(\rho, z) = E_k^+ \eta_k^+(\rho, z),
\]

(3.113)

\[
(\mathcal{L}_{m-s} + X_m) \eta_k^-(\rho, z) = E_k^- \eta_k^-(\rho, z),
\]

(3.114)

where \( E_k^+ \) and \( E_k^- \) are the Hartree-Fock energies. In this basis \( (L_{\pm \pm} + X_{\pm \pm}) \) are diagonal matrices, but it remains to compute the off-diagonal \( X_{\pm \mp} \) exchange operator matrix elements [see Sec. 3.3.1].

Numerical Approach

We wish to solve for Hartree or Hartree-Fock basis modes on a cylindrical grid and we will denote these discretized basis states as \( \eta_k^\pm \rightarrow \eta_k^{[\pm \pm \pm \pm]} \). Here the superscripts denote that the basis states have a total circulation of \( m + s \) and \( m - s \) for the + and − cases, respectively, and also that we are free to choose the z-parity of the excitations. The subscript \( q_{s\pm} \) denotes the order of the radial part of the cylindrical grid, \( k \) labels the excitation and the indices \( i \) and \( j \) denote the radial and axial grid points. We allow for different grid orders for \( \eta^+ \) and \( \eta^- \) since they have different circulations, and as revealed earlier [see Fig. 3.3 and Table 3.2] these may require different grids for the kinetic energy terms to be evaluated accurately. However, since \( m + s \) and \( m - s \) are both either even or odd, we can choose to use a single order for \( q = (m \pm s) \mod 2 \) and obtain accurate results [also see Fig. 3.3 and Table 3.2]. This simplifies our scheme since we do not need to interpolate to take matrix elements between \( \eta^+ \) and \( \eta^- \) functions.

In order to obtain these eigenstates with the Lanczos algorithm we need to act on arbitrary vectors \( f_k^{(\pm \pm \pm \pm)} \) (i.e. sampled on the \( q \)-order cylindrical grid with given \( p_z \) parity) by the relevant operators [left hand side operators of Eqs. (3.111)-(3.114)]. First consider the operator \( \mathcal{L}_{m \pm s} \). As a trivial extension of the ideas used for the GP
operator [see Sec. 3.2.4] we have
\[ L_{m\pm s} [f_{(q)}^{[m\pm s\,ps]}] = \mathcal{T} [f_{(q)}^{[m\pm s\,ps]}] + V [f_{(q)}^{[m\pm s\,ps]}] + V_{H_{(q)}}^{[m\pm s\,ps]} \] (3.115)
where the Hartree potential is
\[ V_{H_{(q)}}^{[0+]} = g_s \left( \psi_{(q)}^{[s+]} \right)^2 + \Phi_{dd}^{[0+]} + \gamma_{QF} \left| \psi_{(q)}^{[s+]} \right|^3. \] (3.116)

The exchange operator Eq. (3.21) can be applied as
\[ X_m [f_{(q)}^{[m\pm s\,ps]}] = \psi_{(q)}^{[spz]} \mathcal{B}^{(m\,q)} \mathcal{F}^{-1} \left[ \mathcal{F}^{[m\pm s\,ps]} \chi_{(m)}^{[mp]\,ps]} \right] + V_{F_{(q)}}^{[0+]} f_{(q)}^{[m\pm s\,ps]}, \] (3.117)
where
\[ \chi_{(m)}^{[mp]} = \mathcal{B}^{(q\,m)} \left( \psi_{(q)}^{[s+]} f_{(q)}^{[m\pm s\,ps]} \right), \] (3.118)
and the (local) Fock potential is
\[ V_{F_{(q)}}^{[0+]} = g_s \left( \psi_{(q)}^{[spz]} \right)^2 + \frac{3}{2} \gamma_{QF} \left| \psi_{(q)}^{[spz]} \right|^3. \] (3.119)
The product of \( f \) (as a proxy for the \( u \) or \( v \) fields) and \( \psi \) can be seen to have circulation of \( m \) from Eq. (3.21), and can be understood by considering the full angular dependence of full 3D functions, i.e. \( \Psi = \psi_s e^{is\phi}, \ u_v e^{is\phi} = u_{mj} e^{i(m+s)\phi}, \ v_{\nu} e^{-is\phi} = v_{mj} e^{i(m-s)\phi} \) [see Eqs. (3.13) and (3.18)], and that the field \( \chi \) arises from the products \( \chi = \Psi^* u_{\nu} \) or \( \chi = \Psi v_{\nu} \), which have total circulation of \( m \).

With the above operators we are able to apply the Lanczos algorithm to obtain the Hartree of Hartree Fock basis \( \{ \eta_{(q)k}^{\pm} \} \) (where we have suppressed circulation and \( z \)-parity for brevity) and associated spectra. In order to obtain the projected BdG matrix \( \mathcal{M}_B \) we need to calculate exchange matrix elements Eq. (3.110). This can be done directly using Eq. (3.117):
\[ (X_{\theta\varphi})_{kk'} = I_r \left[ \eta_{(q)k}^{\theta} X_m \left[ \eta_{(q)k'}^{\varphi} \right] \right], \quad \theta, \varphi \in \{ +, - \}. \] (3.120)

### 3.3.2 Direct BdG Method

Alternatively we can deal with BdG equations directly on the cylindrical grid rather than projecting them onto a basis. However, this requires that we modify the spectrum so that the eigenvalues of interest (those with smallest magnitude) are extremal eigenvalues, rather than existing in the middle of the spectrum, so that we can apply the Lanczos algorithm. Effectively we can do this by squaring the equations. There are two subcases. The first applies to all of the excitations of a \( s = 0 \) (a real, non-vortex
condensate) or to the \( m = 0 \) excitations of a \( s \neq 0 \) condensate, and allows us to reduce the \( 2 \times 2 \) block form of the BdG equations to a single block. This is advantageous because the diagonalization is slower for larger systems. The second and general case does not allow this reduction and we have to deal with the full space.

We will not discuss the \( s = 0 \) case since it is well known in the BEC literature [78]. However, the first case for general \( s \) and \( m = 0 \) the BdG matrix is of the more symmetric form

\[
\mathcal{M} = \begin{pmatrix} \mathcal{L}_s + X_0 - \mu & -X_0 \\ X_0 & -(\mathcal{L}_s + X_0 - \mu) \end{pmatrix}.
\]  

(3.121)

Using the orthogonality transformation

\[
\mathcal{J} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix},
\]  

(3.122)

where \( I \) is the identity matrix, our eigenvalue problem for \( \{u_{0j}, v_{0j}\} \) is orthogonally similar to

\[
\mathcal{H} \begin{pmatrix} x_{0j} \\ y_{0j} \end{pmatrix} = \begin{pmatrix} 0 & \mathcal{L}_s + 2X_0 - \mu \\ \mathcal{L}_s - \mu & 0 \end{pmatrix} \begin{pmatrix} x_{0j} \\ y_{0j} \end{pmatrix} = \epsilon_{0j} \begin{pmatrix} x_{0j} \\ y_{0j} \end{pmatrix},
\]  

(3.123)

where

\[
\mathcal{H} = \mathcal{J}^T \mathcal{M} \mathcal{J},
\]  

(3.124)

\[
x_{0j} = \frac{1}{\sqrt{2}} (u_{0j} + v_{0j}),
\]  

(3.125)

\[
y_{0j} = \frac{1}{\sqrt{2}} (u_{0j} - v_{0j}).
\]  

(3.126)

This allows us to solve the uncoupled equation

\[
(\mathcal{L}_s + 2X_0 - \mu)(\mathcal{L}_s - \mu)x_{0j} = \epsilon_{0j}^2 x_{0j},
\]  

(3.127)

for the square of the eigenvalues. From these solutions \( \{\epsilon_{0j}, x_{0j}\} \) the eigenvectors can be reconstructed using

\[
\epsilon_{0j}^{-1}(\mathcal{L}_s - \mu)x_{0j} = y_{0j},
\]  

(3.128)

\[
\mathcal{J} \begin{pmatrix} x_{0j} \\ y_{0j} \end{pmatrix} = \begin{pmatrix} u_{0j} \\ v_{0j} \end{pmatrix},
\]  

(3.129)
When $m \neq 0$ we cannot perform the above reduction, but we can form system

$$M^2 \begin{pmatrix} u_{mj} \\ v_{mj} \end{pmatrix} = \epsilon^2_{mj} \begin{pmatrix} u_{mj} \\ v_{mj} \end{pmatrix}. \tag{3.130}$$

For real (normalizable) solutions the sign on the eigenvalue can be resolved by taking the expectation of the eigenvectors using $M$. For complex eigenvalues the solutions are zero normalized, but the energy can be computed using

$$\epsilon_{mj} = \frac{\int d^2 x \left| u_{mj} \right|^2 (L_{m+s} + X_m - \mu) u_{mj} - X_m v_{mj}}{\int d^2 x \left| u_{mj} \right|^2}. \tag{3.131}$$

The application of the Lanczos algorithm involves applying the operator either on the left side of Eq. (3.127) or Eq. (3.130) to arbitrary vectors. This requires the parallel and sequential application of the $L$ and $X$ operators presented in Eqs. (3.115) and (3.117), respectively, and requires no further discussion of numerical details.

### 3.3.3 Benchmarking and Comparison of Methods

In general testing of the BdG calculations is involved, and we do not cover the full ranges of tests used in the development of code. However, we note that exact results (such as the trivial zero energy solutions and the Kohn modes) are very useful for ensuring that the calculations are reliable. To date the only published results of excitations of a vortex in a dipolar BEC were given by Wilson et al. in Ref. [79]. In Fig. 3.5 we reproduce calculations presented in [79] (see Fig. 2 in [79]) and find excellent agreement.

In general in many regimes where the DDIs are not too strong (i.e. $\epsilon_{dd} < 1$) and nearly spherical traps, the calculations of BdG excitations are easy to execute and the various methods outlined can all be easily applied to give equivalent results.

However in regimes with strong DDIs or highly anisotropic traps the calculations become more challenging. For example in the flat trap regime with dominant DDIs [such as the results in right side of Fig. 3.5]. Here the interactions vary from being repulsive at small in-plane momentum to attractive at moderate in-plane momentum, and can lead to roton like excitations (e.g. see discussion in [80]). For such cases the basis set methods generally need a large basis ($N_B \gtrsim 10^3$) to get accurate results, where often $N_B \lesssim 10^2$ suffices in near spherical or weak DDI cases. Similarly in the regime of highly elongated trap [81] and self-bound states, the distinct length scales between radial and axial directions complicates the behavior of system. This is the case for the elongated geometry we consider in Ch. 5.
Figure 3.5: Calculation of excitation frequencies of a trapped purely dipolar condensate (i.e. $g_s = 0$ and $\gamma_{QF} = 0$) with a $s = 1$ vortex in a cylindrically symmetric trap with left side figures being $\lambda = \omega_z/\omega_\rho = 2$ and right part being $\lambda = 15$. Plots show (upper plots) imaginary and (lower plots) real parts of the excitation energies as dipole strength increases revealing the emergence of dynamic instabilities. Results are identical to those in [79]. Interaction parameter is $D = 3Na_{dd}/x_0$ where $x_0 \equiv \sqrt{\hbar/m\omega_\rho}$.
Chapter 4

Self-bound Vortex Droplets

In this chapter we present the results of calculations for self-bound vortex droplets, based on the numerical solution techniques we discussed in Ch. 3. We first consider the parameter regime where stationary solutions exist using both full numerical solutions of the extended GPE and the results of a variational Gaussian calculation. We then turn to consider the energetic stability of these self-bound solutions. We find that the vortex solution is always energetically unstable to breaking up into two non-vortex droplets. Our results contradict the original predictions of Cidrim et al. [44] [see Fig. 4.5].

4.1 Self-Bound Vortex Phase Diagram

In the absence of a trapping potential, solutions to the extended GPE (scaled in units of $a_{dd}$ or $a_s$) only depend on two parameters: the number of atoms $N$ and the relative strength of the contact interaction to the DDI, i.e. $\epsilon_{dd}^{-1}$. The trivial solution in this regime is an infinitely dispersed wavepacket of zero density and hence zero energy. For certain parameter regimes it is possible to find self-bound solutions of finite width. These solutions have negative chemical potential, i.e. a tendency to bind more atoms into the self-bound wavepacket, and typically a negative energy\footnote{In some parameter regimes it is possible to find metastable self-bound states with slightly positive energies.}

In Fig. 4.1 we show some examples of self-bound (and a trap bound) vortex droplet for dysprosium parameters. We observe that the self-bound solutions tend to be highly elongated along the direction that the dipoles are polarized (i.e. $z$-axis). This allows them to minimize the DDI energy since in this geometry most of the DDIs are of the attractive head-to-tail type [see Fig. 2.2(d)]. Self-bound droplets can only exist for $\epsilon_{dd} > 1$, and with sufficiently many atoms. This was also found for the case of non-vortex dipolar droplets in [36]. The comparison of the vortex and non-vortex droplets [see Fig. 4.1(a)], reveals that they can have a significant difference in their spatial extents. This arises because the vortex core takes up a large fraction of the droplet
Figure 4.1: (a) Droplet density isosurfaces for a (left) \( s = 0 \) stationary state and (right) \( s = 1 \) vortex droplet. Red, green and blue colour surfaces are the at 0.9, 0.7 and 0.5 of the peak density, respectively, with \( N = 12 \times 10^3 \) Dy atoms, and \( \epsilon_{dd} = 2 \). For the stationary state \( \mu = -2.6 \) kHz, \( E/N = -2 \) kHz, while for the vortex state \( \mu = -1.4 \) kHz, \( E/N = -0.52 \) kHz, where \( E/N \) is the total energy per particle. (b) Density plot of vortex droplets for various values of \( \epsilon_{dd} \), and \( N = 12 \times 10^3 \) atoms (note logarithmic colour scale). No trap potential is presented (i.e. droplets are self-bound), except for last result with spherical trap \( \omega/2\pi = 70 \) Hz.

In general the droplets become smaller and denser as \( \epsilon_{dd} \) increases. The droplets are unable to self-bind for \( \epsilon_{dd} \leq 1 \), where the repulsive contact interaction is able to always dominate over the attractive component of the DDI. The last subplot in Fig. 4.1(b) shows a result at \( \epsilon_{dd} = 1 \) where a trap is needed to bind the condensate (i.e. this is a standard trapped dipolar BEC rather than a droplet). We observe that as \( \epsilon_{dd} \to 1 \) the energy and chemical potential of the self-bound droplets get less negative.

We can construct a phase diagram for the regimes where self-bound stationary states can be found. The coloured regions in Fig. 4.2 show where negative energy solution of the variational gaussian [Eqs. (2.24) and (2.25)] \(^{36, 45} \) for non-vortex \((s = 0, \) pink region\) and vortex \((s = 1, \) blue region\) can be found. The non-vortex results correspond to those presented in Ref. \(^{36} \) and the vortex region was presented by Cidrim et al. in Ref. \(^{45} \). For reference we have also indicated the parameters of the states shown in Fig. 4.1(b) as diamonds on the phase diagram [see Fig. 4.2]: The black diamonds with white filling indicate the self-bound vortex states, while the red filled diamond indicates the trapped case which is seen to lie outside where self-bound states
are predicted to exist. We have also added the results of full GPE calculations for the stability boundary (pink and blue circles). These results were obtained for fixed $N$ by increasing $\epsilon_{dd}^{-1}$. As this happens the droplet tends to get bigger and eventually, for large enough $\epsilon_{dd}^{-1}$, we are unable to find a converged stationary solution. We identify the last converged numerical solution as the GP boundary point.

![Phase diagram for where $s = 0$ non-vortex (pink shaded region) and $s = 1$ vortex (blue shaded region) self-bound droplets exist. We mark the last points of our full GPE numerical calculation as hollow circle. The four solutions in Fig. 4.1(b) are denoted with diamonds.](image)

**Figure 4.2:** Phase diagram for where $s = 0$ non-vortex (pink shaded region) and $s = 1$ vortex (blue shaded region) self-bound droplets exist. We mark the last points of our full GPE numerical calculation as hollow circle. The four solutions in Fig. 4.1(b) are denoted with diamonds.

### 4.2 Vortex Droplet Properties

We can also examine various properties of the self-bound vortex droplet solutions as parameters vary. Such a study was presented in Cidrim et al. in Ref. [45], and we choose to examine the same parameter regime to compare our calculations. The quantities they considered were the vortex core width and the droplet widths. The vortex core width was obtained by integrating the density along $z$, and finding the length over
which this column density increase from 10% to 90% of its peak value. The droplet widths were defined by the moments (chosen to be compatible with the variational widths defined in the Gaussian ansatz [see Eqs. (2.22) and (2.23)])

\[
\sigma_{\rho} = \sqrt[4]{\frac{1}{\sqrt{\pi}} \rho |\psi(x)|^2 dx}
\]

(4.1)

\[
\sigma_{z} = \sqrt{\int \frac{8}{3} z^2 |\psi(x)|^2 dx}.
\]

(4.2)

In Fig. 4.3, we present our results indicating the peak droplet density and the various widths for droplets. For comparison, the final results of Cirdim et al. in Ref. [45] are shown in Fig. 4.4. We notice that Cidrim results have appreciable scatter in their predicted width values as \(\epsilon_{dd}^{-1}\) varies, while ours are smooth. Note, because the \(y\)-axis is logarithmic on these graphs this scatter is indeed significant, and suggests their calculations were not converged. Notable, their core width for the case of \(N = 10^5\) is seen to change abruptly at \(\epsilon_{dd}^{-1} \sim 0.2\), which is a feature we do not see. The results in the earlier preprint [44] had even more significant scatter in the results, so one can see that they have improved their numerics for the final version although it appears some issues still remain in their calculations. Most notably, they do not mention any use of a cutoff DDI potential, while our results in Ch. 3 [see Table 3.2] indicate that the proper use of a cutoff DDI potential was essential to ensure accurate results.

Figure 4.3: Our calculations of (a) the peak density, (b) the vortex core width, and (c) the vortex droplet widths. Results of GPE calculations shown as symbols, compared to variational gaussian results solid and dashed lines. Dash and solid lines in (c) are related to width of \(\sigma_z\) and \(\sigma_\rho\), respectively.

The peak density [see Fig. 4.3(a)], and to a lesser extent the vortex core width [see Fig. 4.3(b)], is seen to converge for independent of \(N\) for strong DDIs (i.e. small \(\epsilon_{dd}^{-1}\)). The peak density behaviour is expected because the droplet should become incompressible with a density set by the balance of two-body interactions with quantum
fluctuations, and more atoms will just cause the droplet to be larger. In such a regime it is not surprising that the vortex core will also become universal. We also observe that the full GPE solutions show a closer collapse towards the same density at strong DDIs related to the variational solution. This indicates that the variational solution, which always has a Gaussian profile and cannot exhibit a saturated density profile, is becoming a poor approximation in this regime.

4.3 Energetic Stability

Finally we consider the energy stability of a self-bound vortex. In general we expect that for a droplet with \( N \) atoms to be stable it should have a lower energy than two droplets with \( N/2 \) atoms. This is the case for non-vortex droplets in free-space, where \( E/N \) decreases as \( N \) increases. However, for a vortex case we can ask if a vortex droplet of \( N \) atoms has lower energy than two non-vortex droplets of \( N/2 \) atoms. This is motivated by the observation of a vortex droplet dissociating into two non-vortex droplets in time dependent simulations [e.g. see Fig. 1.7].

To explore this we consider the energy difference

\[
\Delta E = E_1(N) - 2E_0(N/2),
\]

where \( E_1(N) \) is the energy of a \( s = 1 \) vortex droplet with \( N \) atoms and \( E_0(N/2) \) is the energy of a \( s = 0 \) non-vortex droplet with \( N/2 \) atoms. When \( \Delta E > 0 \) the vortex droplet can be considered unstable. However, this argument does not take into account the angular momentum of the vortex, thus the dissociation must occur such that the fragment droplets emerge with some kinetic energy or excitation to conserve
the angular momentum.

In the first preprint Cidrim et al. [44] significantly predicted that for large \(N\) and strong DDIs \(\Delta E\) could be negative. We show this result in Fig. 4.5(a). Notable for \(N = 10^5\) and \(\epsilon_{dd}^{-1} \lesssim 0.3\) they find \(\Delta E < 0\). This prediction was also supported by the Gaussian variational result, which also becomes negative for these parameters. However, the scatter on their results is severe, questioning the reliability of their results. Also, as noted in our discussion of the density predictions for self-bound droplets in Sec. 4.2, the Gaussian variational results is expected to become unreliable in this regime, particular when calculating a quantity related to the difference of two energies.

Our high accuracy results for \(\Delta E\) are shown in Fig. 4.5(b), and reveal that \(\Delta E\) is positive. This indicated the essential role of high accuracy numerical calculations for dipolar system, and in particular careful treatment of the DDI. We note that in the final published version of the Cidrim paper this result was removed.

![Figure 4.5: The energy of a self-bound vortex with \(N\) atoms relative to two (non-vortex) droplets each with \(N/2\) atoms. A negative energy indicates that the vortex has a lower energy and is thus energetically stable. Subplot (a) shows the results of the preprint Ref. [44]. Here the GPE calculations are circles, and the solid lines are from the variational solution. Subplot (b) shows our GPE results. The energy units are \(Nh^2/Ma_{dd}^2\), where \(g_{dd} \equiv 4\pi a_{dd}^2h^2/M\).](image)

Figure 4.5: The energy of a self-bound vortex with \(N\) atoms relative to two (non-vortex) droplets each with \(N/2\) atoms. A negative energy indicates that the vortex has a lower energy and is thus energetically stable. Subplot (a) shows the results of the preprint Ref. [44]. Here the GPE calculations are circles, and the solid lines are from the variational solution. Subplot (b) shows our GPE results. The energy units are \(Nh^2/Ma_{dd}^2\), where \(g_{dd} \equiv 4\pi a_{dd}^2h^2/M\).
Chapter 5

Excitations of a Vortex Line in an Elongated Dipolar Condensate

In this chapter we characterise the properties of a vortex line in an elongated dipolar Bose-Einstein condensate. We start by increasing the strength of the dipole-dipole interactions (DDIs) relative to the short ranged contact interactions. We then find that the system crosses over to a self-bound vortex droplet stabilized from collapse by quantum fluctuations. Following from that, we calculate the quasiparticle excitation spectrum of the vortex state, which is important in characterizing the vortex response, and assessing its stability. When the DDIs are sufficiently strong we find that the vortex is dynamically unstable to quadrupolar modes. Most of the results in this chapter have been published in PRA [47].

5.1 Introduction to the Elongated Dipolar Condensate

In this section we demonstrate the properties of collective modes in a dipolar condensate with a vortex line [e.g. see Fig. 5.1]. For condensates with short ranged (contact) interactions such a vortex line has been prepared by rotating a cigar shaped trap about its axis of symmetry [82]. In that system Kelvin waves [e.g. see Fig. 5.1(a)] were observed, emerging from a parametric resonance with a quadrupolar excitation that could be directly driven with a rotating perturbation [83] (also see [84, 81, 85]). To date there has been no reported observation of vortices in a dipolar condensate, however there has been considerable theoretical interest in this topic (e.g. [86–97]). Notably, Klawunn et al. [91, 93] found that the DDIs affected the Kelvin modes of a vortex line, and that for negatively tuned DDIs the Kelvin dispersion relation could develop a roton-feature leading to a transverse instability of the vortex line.

As we mentioned in Ch. 1, the recent observation of quantum droplets formed from
a dipolar condensate have opened new directions of research in this system. These droplets occur for sufficiently strong DDIs and arise from the interplay of attractive two-body interactions and the repulsive quantum fluctuation (QF) effects [24, 29–33, 36, 37]. Irrespective of their confinement, dipolar quantum droplets tend to have an elongated (prolate) density distribution with the long axis in the direction that the dipoles are polarized. Recently Cidrim et al. [45] which had been discussed in Ch. 4 considered whether these droplets might be able to support a vortex. They presented predictions for vortex droplet stationary states, but observed that under time evolution these states were highly unstable with a tendency to split into two parts.

Figure 5.1: Density isosurface of the $s = 1$ vortex state of a condensate for (a) purely contact interactions and (b) a dipole interaction strength close to instability. In subplot (a) a Kelvin-wave quasiparticle is superimposed on the condensate causing the vortex line to wiggle [mode (k) indicated in Fig. 5.4(a)]. In subplot (b) a quadrupolar quasiparticle is superimposed on the condensate causing the density around the vortex to split into two pieces [mode ($q_3$) indicated in Fig. 5.4(d)]. Isosurfaces indicate a density of $10^{20}$ m$^{-3}$. 
The primary system we consider in this chapter is an elongated dipolar condensate confined in a prolate harmonic trap with a vortex line on its long axis. We use extended meanfield theory showed in Ch. 3 to calculate stationary vortex states. We find that for the trap geometry we consider, the condensate continuously transforms into a vortex droplet as the DDIs increase in strength relative to the contact interactions, thus demonstrating a viable scheme for producing vortex droplets.

We also solve the Bogoliubov-de Gennes equations showed in Ch. 3 for the quasi-particle excitations. This allows us to quantify the effect of the DDIs and QFs on the Kelvin wave modes, and other relevant low energy modes, and to assess the origin of dynamical instabilities in the system. We find that the first strong instabilities to emerge are quadrupolar in character, causing the condensate to break into two pieces [e.g. see Fig. 5.1(b)], consistent with the decay dynamics seen in Ref. [45]. By turning off the QF term in the generalized meanfield theory we can assess the effect of this term on stability and the excitation spectrum of the system. Our results show that the QF terms can have marked differences in the spectral properties, even before the system is in the droplet regime. Furthermore, comparison of our results to experiments or alternative theories may be useful in establishing the accuracy of the QF term (in the local density approximation) for vortex states.

The main results of this chapter are presented in Sec. 5.2. We begin by examining the stationary state properties, and the crossover to the vortex droplet state as the DDIs increases (with the QF term) or the mechanical collapse of the condensate (without the QF term). We then present the related excitation spectrum focusing on the low energy branches and identify the modes that cause the vortex to become dynamical unstable.

The numerical solution of Eq. (3.19) for the case of vortex stationary states is reasonably challenging, and details of our approach have been already discussed in Ch. 3. For further discussion on the numerical methods, an even more thorough study is planning in the near future.[98].

### 5.2 Numerical Results

For our calculations we take $N = 112 \times 10^3$ $^{164}$Dy atoms in a cigar shaped trap with $\omega_{\perp} \gg \omega_z$ (Note that we change the notation of radial trap frequency from $\omega_p$ in earlier chapters to $\omega_{\perp}$ in this chapter), choosing the case $(\omega_{\perp},\omega_z)/2\pi = (98.5, 11.8)$ Hz to match the trap used in Ref. [83], and taking a scattering length of $a_s = 80 a_0$, where $a_0$ is the Bohr radius.
5.2.1 Stationary State Properties

We present our results for the condensate properties in Fig. 5.2 as a function of the DDI strength, parameterized by the dipole length $a_{dd}$. The strength of the DDI can be tuned using a rotating magnetic field [99, 53] [see Sec. 2.2.1] up to the maximum value (in a static field) of $a_{dd} = 131 a_0$ for $^{164}$Dy [see Table 2.1].

In the absence of the QF term the system becomes mechanically unstable to collapse, where the condensate widths are seen to decrease and the density increases rapidly as $a_{dd}$ increases towards $a_{dd} \approx 85 a_0$ [e.g. see Figs. 5.2(a) and (b)]. Because the DDIs are anisotropic this type of collapse instability is dependent on the geometry of the system [100, 26]. Since our trap arranges the condensate into a prolate shape (which enhances the attractive head-to-tail part of the DDI), collapse occurs soon after the interactions become dipole dominated (i.e. when $a_{dd} > a_s = 80 a_0$).

Including the QF term [see magenta line in Fig. 5.2] stabilizes the system against mechanical collapse, and the condensate density grows more slowly as $a_{dd}$ increases. In the regime $a_{dd} > 85 a_0$ (where collapse would occur without the QF term) the system crosses over to a quantum droplet, and then becomes self-bound (i.e. can maintain itself as a localized structure even in the absence of confinement [36, 37]). We can illustrate this by considering the system chemical potential and energy [Figs. 5.2(c) and (d)], which both become negative for $a_{dd} \gtrsim 120 a_0$, indicating that the state is self-bound [36, 38]. Here the energy is calculated using the energy functional Eq. (2.12). We can also compare the trapped solutions to free space self-bound solutions, i.e. stationary solutions of Eq. (2.8) with $V_{tr} = 0$ [45, 36]. These results are shown as green curves in Fig. 5.2 and confirm that the trapping potential plays a minor role in the stationary state properties for sufficiently large $a_{dd}$ values.

It is more convenient for experiments to tune $a_s$ using a Feshbach resonance, keeping $a_{dd}$ fixed. We have repeated the type of stationary state analysis presented in Fig. 5.2 but fixing $a_{dd} = 131 a_0$ and varying $a_s$ [see Fig. 5.3], i.e. starting from an initial value $a_s > a_{dd}$ and then decreasing $a_s$ to bring the system into the regime of dominant dipole interactions. For this case we find that without the QF term the vortex state is unstable to mechanical collapse at $a_s \lesssim 124 a_0$. With the QF terms the system smoothly crosses over to a vortex droplet attaining a negative chemical potential and energy for $a_s \lesssim 90 a_0$. Similar behavior has been observed in experiments [30], where a droplet was prepared in a prolate trap geometry, albeit for a non-vortex ($s = 0$) case and by reducing $a_s$. It is not expected that this behavior will persist in traps with oblate geometries where the droplet state and the condensate do not smoothly connect (see [101, 33, 102]).

We also show results for the energy $E_0$ of the respective $s = 0$ ground states in Fig. 5.2(d). In a non-rotating reference frame these states have a lower energy compared to the vortex states when they exist. However we note that the ground state
Figure 5.2: Comparison of trapped condensate properties with (magenta lines) and without (blue lines) QF corrections as $a_{dd}$ varies. Free space self-bound droplet solutions (green lines) are also shown. (a) Peak density $n_{\text{peak}} = \max(\psi_s^2)$ of the $s = 1$ condensate. (b) Condensate widths given by the rms expectations of the $x$ (dotted) and $z$ (solid line) coordinates. (c) Chemical potential and (d) energy per particle of the $s = 0$ ground state (dashed lines) and $s = 1$ vortex state (solid lines). Inset to (d): The thermodynamic critical rotation frequency for the $s = 1$ vortex state. The dotted horizontal line indicates the radial trap frequency for reference.
Figure 5.3: Figure comparing between different properties of condensates in the same format as Fig. 5.2, but the parameter changing along x-axis is now being $a_s$ while fixing $a_{dd} = 131a_0$. 
for $\gamma_{QF} = 0$ collapses at a lower value of $a_{dd}$ than the vortex state, thus there is a small range of $a_{dd}$ values where $E_1$ can be calculated yet $E_0$ is undefined. The energy difference between the $s = 0$ and $s = 1$ states relates to the thermodynamic critical angular frequency $\Omega_c$:

$$\Omega_c = \frac{E_1 - E_0}{Nh}, \quad (5.1)$$

where $\Omega_c$ is the rotation frequency about the $z$ axis required for the vortex state to become energetically favorable. Our results for $\Omega_c$ [see inset to Fig. 5.2(d)] show that $\Omega_c$ increases with $a_{dd}$. This behavior was expected for a prolate dipolar condensate within the hydrodynamic approximation [90, 95] (cf. [94]). For results including the QF term in the droplet regime the critical rotation frequency can exceed the radial trap frequency (i.e. for $a_{dd} \gtrsim 95a_0$). We note that the self-bound result (green) terminates at $\Omega_c \approx \omega_{\perp}$ by coincidence for this choice of interaction parameters.

5.2.2 Excitation Spectrum

In Fig. 5.4 we present the results for the quasiparticle excitation spectra corresponding to stationary states analyzed in Fig. 5.2 for various $a_{dd}$ values, both with and without the QF term. We restrict our attention to excitations with relative angular momentum quantum number $|m| \leq 4$, which are the lowest energy excitation branches, with higher angular momentum excitations beginning at energies above the range we consider. Our primary focus is on the $m = 0, -1, -2$ branches which we discuss further below. Subplots (d) and (f) show the excitation spectra for $a_{dd}$ close to dynamical instability (i.e. where the excitation energies develop imaginary parts) for the cases with $\gamma_{QF} = 0$ and $\gamma_{QF} \neq 0$, respectively. The imaginary parts of the spectrum are shown in Figs. 5.4(α) and (β) as a function of $a_{dd}$, revealing that the first dynamically unstable modes develop at $a_{dd} \approx 82.5a_0$ for $\gamma_{QF} = 0$ and at $a_{dd} \approx 94a_0$ when we include the QF term.

To visualize the spectra we follow the procedure introduced in Ref. [81] to map the excitations on to an effective dispersion relation as a function wavevector $k_z$ along the vortex line. This is done by ascribing an average axial wavevector to each excitation according to

$$\langle k_z \rangle_{m_j} \equiv \sqrt{-\int dx u^*_{m_j} \frac{\partial^2}{\partial z^2} u_{m_j} \int dx |u_{m_j}|^2}. \quad (5.2)$$

1We emphasize that $\Omega_c$ is the critical frequency required to make the $s = 0$ and $s = 1$ states energetically degenerate, and does not mean that the $s = 1$ state is necessarily dynamically stable when it is rotated at $\Omega_c$.

2The results of Fig. 5.4(α) are approximately comparable to Fig. 3 of Ref. [81], although the larger mass of Dy introduces a scaling of the $k_z$-axis.
Figure 5.4: (a)-(f) Quasiparticle excitations of an \( s = 1 \) vortex with \( -4 \leq m \leq 4 \) are shown for various \( a_{dd} \) as indicated in each plot. Subplots (a)-(d) show results without QF corrections, while (e) and (f) include QF corrections. The parity of excitations along \( z \) is even (circles) or odd (triangles). The solid lines are dispersion relation fits [see text, and Eqs. (5.3) and (5.5)] and the horizontal dotted line indicates \( -\Omega_c \) [also see inset to Fig. 5.2(d)]. Subplots (α) and (β) show the imaginary parts of dynamically unstable modes. The labels (k) and (q1) to (q5) identify modes we discuss in the text [also see Figs. 5.1 and 5.6].

With this mapping we see that the excitations in Figs. 5.4(a)-(f) mostly lie on reasonably smooth curves. Due to finite size effects of the trapped system, some modes fall below these smooth curves. For an example consider the lowest 2 pairs of \( m = -1 \) “bending” modes in Fig. 5.4(a). These modes have been analyzed in detail in prior work (see Ref. [81]), and are surface Kelvin modes that have most of their amplitude near the top and the bottom of the condensate.

We can arrive at a simple model for the \( m = 0 \) phonon branch based on the assumption that the condensate and excitations have a Gaussian radial profile of the form \( \chi(\rho) = l_{\rho}^{-1} e^{-\rho^2/2l_{\rho}^2 + i\phi}/\sqrt{\pi}l_{\rho} \) (Note the \( \chi \) here is different to what we defined in Ch. 3), which has a maximum at \( \rho = l_{\rho} \). For a system that is uniform in \( z \), we obtain
the dispersion relation \[38, 104\]

\[\epsilon_{k_z} = \sqrt{\epsilon_0^2 + 2\epsilon_0 n_{\text{peak}} c_f \left\{ g_s - g_{dd} F_X \left( \frac{k_z l_p}{\sqrt{2}} \right) + c_{\text{QF}} \gamma_{\text{QF}} n_{\text{peak}}^{1/2} \right\}}, \] (5.3)

where \(\epsilon_0 = \hbar^2 k_z^2 / 2M\), \(c_{\text{QF}} = \frac{18}{25} \sqrt{\frac{2\pi e}{5}} \approx 1.33\),

\[F_X(q) = 1 + \frac{3}{2} q^2 \left[ (q^2 + 2)^2 e^{q^2} \text{Ei}(-q^2) + q^2 + 3 \right], \] (5.4)

with Ei being the exponential integral, and \(n_{\text{peak}}\) being the peak density. This result can be applied to our case taking \(l_p\) as the radius at which the condensate density is maximum in the \(z = 0\) plane. We have left \(c_f\) as a fit parameter\(^3\) that accounts for the spatially varying density along \(z\), and for our fits, \(c_f\) varies from 0.14 to 0.38, which is comparable to a similar factor used in Ref. [81]. In Fig. 5.4(d) the phonon dispersion curve provided by Eq. (5.3) starts at finite \(k_z\) (just visible near \(k_z = 0\)) because it is imaginary (dynamically unstable) for smaller \(k_z\) values, suggesting that the trapped system is stable in this regime due to finite size effects (i.e. no phonon mode exists with long enough wavelength to access the instability).

We observe that the phonon spectrum changes appreciably as \(a_{dd}\) increases, notably changing from being linear to having curvature and growing more rapidly over the range considered. We note that \(\mu\) [see Fig. 5.2(c)], and hence the speed of sound \(c = \sqrt{\mu/M}\), decreases with increasing \(a_{dd}\). The speed of sound corresponds to the slope of the dispersion curves in \(k_z \to 0\) limit. The fitted phonon dispersion lines Eq. (5.3) indicate that this slope does decrease with increasing \(a_{dd}\), although the first discrete excitation in this branch occurs at a \(k_z\) value beyond where the linear behavior holds, i.e. the curvature in the dispersion is already important. This curvature originates from the momentum dependence of the DDIs in the elongated geometry: excitations with \(|k_z l_p| < 1\) experience an attractive DDI that reduces the value of \(\epsilon_{k_z}\), while excitations with \(|k_z l_p| > 1\) experience a repulsive interaction that increases \(\epsilon_{k_z}\). This behavior is described by the \(-g_{dd} F_X\) term in Eq. (5.3).

The \(m = -1\) excitation branch corresponds to Kelvin waves of the vortex line [e.g. see Fig. 5.1(a)]. To fit the Kelvin spectrum we use the dispersion relation introduced by Simula et al. [81] (also see [105, 106])

\[\omega(k_0 + k_z) = \omega_0 + \frac{\hbar k_z^2}{2M} \ln \left( \frac{1}{|r_c k_z|} \right), \] (5.5)

valid for \(|r_c k_z| \ll 1\), where \(r_c\) is the so called vortex core parameter. Following Ref. [81] we take \(r_c\), \(k_0\) and \(\omega_0\) as a fitting parameters. In the case of contact interactions the

\(^3\)For a vortex that is uniform along \(z\), and takes the prescribed Gaussian form radially, we have \(c_f = e/4 \approx 0.68\).
core parameter was found to be weakly dependent on system parameters, even when the healing length changed appreciably (see [81, 85, 105]). For our fits (presented in Fig. 5.4), we find that \( r_c \) changes significantly to accommodate the stiffening of the Kelvin mode excitation branch as \( a_{dd} \) increases. E.g., \( r_c \) changes from 0.12\( \mu \)m in Fig. 5.4(a) to 0.02\( \mu \)m in Fig. 5.4(d). This stiffening of the Kelvin mode behavior was predicted for a vortex line in a uniform dipolar condensate in [91] and given a simple interpretation: The density core in the vortex line can be viewed as a set of holes that effectively interact with each other via the DDI. For \( a_{dd} > 0 \) these holes minimize energy in a straight line configuration (i.e. in an attractive head to tail arrangement). The Kelvin modes cause the vortex line to wiggle [e.g. see Fig. 5.1(a)] incurring an energy cost from the repulsive (side-by-side) component of the DDI, hence causing the Kelvin mode energy to increase with increasing DDI strength.

We find in Figs. 5.4(\( \alpha \)) and (\( \beta \)) that the \((m = -1)\) Kelvin mode energies can develop an imaginary part for sufficiently large \( a_{dd} \) values. Often the magnitude of this imaginary part remains small [see Fig. 5.5], so that these modes are weakly unstable, and will grow slowly. Also the dynamic instability of these modes oscillates as \( a_{dd} \) changes. Similar behavior has been seen in other work considering excitations of vortices (e.g. see [107, 92, 108]), and was found to arise from the coupling of modes that are crossing each other as a parameter is changed (e.g. see Fig. 4 of [109]). This suggests that the Kelvin modes will not strongly grow, but that there is a tendency for the vortex line to wobble. We note that for the case without the QF term [see Fig. 5.4(\( \alpha \))], a pair of Kelvin modes grow to have a large imaginary part for \( a_{dd} \gtrsim 84 a_0 \), but this occurs well after an \(|m| = 2\) mode has developed as a strong instability.

Finally, we consider the \( m = -2 \) excitation modes, which have a quadrupolar character. As \( a_{dd} \) increases, these modes tend to lower their energy relative to the other branches, and notably near instability [see Figs. 5.4(d) and (f)] some of these modes have negative energy. Figs. 5.4(\( \alpha \)) and (\( \beta \)) reveal that the \(|m| = 2\) modes are the first to develop large imaginary energies both with and without QFs. This suggests that quite generally the quadrupolar modes will drive the instability of the dipolar vortex line.

To understand the onset of instability we consider the density perturbation associated with the unstable modes. The density perturbation \( \delta n_{mj} \) is the leading order change in the condensate density when we add an \( \{mj\} \)-quasiparticle to the condensate and is given by

\[
\delta n_{mj} = \psi_s(u_{mj} - v_{mj}).
\]  

(5.6)

In Fig. 5.6 we plot \( \delta n_{mj} \) for the lowest energy \( m = -2 \) mode, which is the first quadrupolar mode to become dynamically unstable. The mode shown is identified as (q1) to (q5) for the different parameter sets and is labeled in Fig. 5.4 for reference.
Well before instability [i.e. (q1) for $\gamma_{QF} = 0$ and (q4) for $\gamma_{QF} \neq 0$] the lowest energy quadrupolar mode exists at the surface (top and bottom) of the condensate, and the fluctuation affects the density in these regions. These modes have negligible tunneling through the condensate so that the even and odd $z$-parity modes are degenerate [see Fig. 5.4]. We observe that other degenerate pairs of surface modes often exist, while the rest of the $m = -2$ branch excitations are non-degenerate and fall on a smooth effective dispersion curve.

For the $\gamma_{QF} = 0$ case close to instability [see Fig. 5.4(c)] the degeneracy is broken between the odd and even modes as the excitation extends through the bulk of the condensate [see Fig. 5.6(q2)]. The energy of this mode descends quickly with increasing $a_{dd}$ as we move closer to instability [see Fig. 5.4(d)] and the magnitude of the density fluctuation increases significantly [see Fig. 5.6(q3)]. This occurs because the $v$-amplitude changes phase relative to the $u$-amplitude (which also indicates that the excitation is experiencing an effective attractive interaction), thus enhancing $\delta n_{mj}$.

In Fig. 5.1(b) we indicate the density pattern of the condensate with the (q3) mode coherently added, seeing that this perturbation tends to split the condensate into two parts.

The case with $\gamma_{QF} \neq 0$ progresses towards instability in a similar manner. The degeneracy and hence the top and bottom surface character of the lowest $m = -2$ modes persists to higher values of $a_{dd}$ [see Fig. 5.4(e) and Fig. 5.6(q4)], but eventually breaks
Figure 5.6: Density fluctuations $\delta n_{mj}$ of various even $z$-parity (q1)-(q5) $m = -2$ and (q1')-(q5') $m = 2$ quadrupolar modes [as labeled in Figs. 5.4(b)-(f)]. For reference the white lines indicate a contour of the condensate density at 0.1 of its peak value. Subplots (a) and (b) show the $m = -2$ spectrum, including positive norm (green), negative norm (purple) and the dynamically unstable (orange) modes. Both even (solid line) and odd (dashed line) $z$-parity modes are shown. The (q1)-(q5) mode energies are indicated with small circles. The negative norm (q1)-(q5) mode energies are the negative of the energies for the corresponding positive norm modes for $m = 2$ [see Ch. 3]. Using this correspondence we also indicate the (q1')-(q5') mode energies on these subplots with small circles.

when the surface modes again extend into the bulk [see Fig. 5.4(f) and Fig. 5.6(q5)].

In Figs. 5.6(a) and (b) we see that the dynamic instability occurs when a positive norm and a negative norm quasiparticle mode in the same subspace collide (also see 107, 109, 110). As we discussed in Sec. 3, a negative-norm mode in the $m$-subspace is equivalent to a positive-norm mode in the $-m$-subspace (albeit with an inverted energy sign). Thus the emergence of a dynamically unstable mode in the $m = -2$ subspace will have a partner excitation in the $m = 2$ subspace that it will collide with. In subplots (q1') to (q5') of Fig. 5.6 we show the $m = 2$ excitation that partners with the $m = -2$ mode shown in (q1)-(q5).

It is worth taking a step back to consider the behavior of the quadrupole modes,
prior to their instability, in terms of the various energy contributions. The kinetic energy cost of the azimuthal phase winding differs between the two quasiparticle amplitudes in Eq. (3.13), being proportional to \((m + s)^2\) for the \(u_{mj}\) amplitude, and \((m - s)^2\) for the \(v_{mj}\) amplitude [see Eqs. (3.19), (3.18), (3.6) and (3.7)]. For \(m = -2\) excitations, this places a greater energy cost on the \(v_{mj}\) amplitude as compared to \(u_{mj}\). As a consequence, far before the instability the relevant \(m = -2\) excitations are strongly confined to the top and bottom ends of the condensate [Figs. 5.6(q1) and (q4)], minimizing \(|v_{mj}|\) by reducing their overlap with the condensate. In contrast, for the partner \(m = 2\) excitations [Figs. 5.6(q1')] and (q4')] the energy bias is reversed and the energy is reduced by maximizing \(|v_{mj}|\), i.e. the excitation extends throughout the bulk of the condensate. However, even for \(m = 2\) the \(u_{mj}\) terms still dominates and the density perturbations shown in [Figs. 5.6(q1')] and (q4')] clearly exhibit the effects of its larger centrifugal energy, pushing the excitation radially further outwards. Eventually, for increasing \(a_{dd}\) the attractive component of the DDI starts to dominate and the \(m = \pm 2\) partner excitations begin to hybridize as they approach their instability. As a result, the \(m = -2\) excitations overcome their high-density aversion and extend into the bulk of the condensate. The increased tunnelling between the two ends destroys the energetic degeneracy of the odd and even \(z\)-parity modes.
Chapter 6

Conclusion

In this final chapter we summarize our results for the elongated dipolar Bose-Einstein condensate with a single charge vortex. We also talk about the future prospects emerging from this work.

6.1 Result

The major technical challenge of this thesis was to produce the first numerical algorithms and efficient code for computing the excitations of dipolar vortex droplets. As is apparent in chapter 3, great care is needed with the choice of quadrature, regularized dipole-dipole interaction potential, appropriate use of specialized Bessel interpolation to ensure accurate results. This arises because for the case of a vortex the $u$ and $v$ excitations occur with different relative angular momentum and on face value require different quadratures. However, we have found that it is possible to greatly simplify the problem, with no loss of accuracy, by the appropriate choice of a 0- or 1-order Bessel grid for the radial direction. Similarly, by employing a type-IV discrete cosine or sine transformation we can make use of the axial symmetry of the problem while using identical quadrature grids for each axial symmetry class. Indeed, it took the majority of this research to arrive at an efficient and accurate algorithm, and to implement this in code. The excitation calculations are much more time consuming than the ground state calculations. Particularly in the dipole dominated regimes of interest the Lanczos algorithm requires a large number of iterations to converge, hence making our efficient use of quadrature and grids (via the cutoff interaction potential) is an essential development.

The original motivation of our work came from a preprint that appeared on self-bound vortex droplets. Using our tools we have improved on the results in that work, confirming that they incorrectly predicted energetic stability of these droplets due to issues with their numerical calculations.

We have used our computation tools to explore the properties of a vortex line in an
elongated dipolar Bose-Einstein condensate. We have presented results for the system properties as the DDI strength is changed, observing that the system smoothly evolves from being a trap bound vortex into a self-bound vortex droplet as the strength of the DDI interaction increases. We have also presented results for the quasiparticle excitation spectrum of the system, revealing the behaviour of the Kelvin wave and other low energy excitations. In the regime of dominant DDIs we find that this system becomes dynamically unstable to quadrupolar excitations, which appears to be consistent with the decay dynamics observed in GPE simulations of vortex droplets [45]. More generally, our work suggests that vortices in dipolar droplets are unstable (i.e. have a short lifetime), cf. vortices in binary mixture droplets [111].

We have presented our results both with and without QFs to reveal their effects on the system. Of course the QFs are necessary for droplet formation at high values of the DDI, but also we observe differences even before this regime [for example in the $m = -2$ excitation modes at $a_s = 80 a_0$, compare Figs. 5.4 (c) and (e)]. Such excitations might be accessible to direct driving (e.g. see [83]) or could be probed with Bragg spectroscopy using light fields that carry angular momentum (cf. [112–114]). This kind of study would also be useful for gaining a better understanding of the accuracy of the QF treatment we use here which is based on the local density approximation.

Experiments have yet to report the observation of vortices in a dipolar condensate. Increased understanding of this system and the regimes where dynamic instabilities occur will be important in future experimental studies.

6.2 Future Outlook

To finish we briefly comment on a few directions that could follow on from our work.

- Non-dipolar binary condensates can also form droplets (see [43]), and it has been shown that these can support vortices in appropriate parameter regimes [111]. However, such regimes do not look accessible to current experiments with $^{39}$K. Recently the first dipolar binary BEC system has been produced in experiments as a mixture of erbium and dysprosium atoms [115], and it may be that binary dipolar system forms droplets with different properties, e.g. lower densities, less elongated into filaments. This appears to be a promising system for exploring the existence of stable self-bound vortices.

- In this thesis we have focused on finding excitations for a condensate in a prolate trap where the system transforms smoothly into a droplet. It will be interesting to consider nearly spherical or oblate shaped traps. In the latter case the transition is expected to be first order in character, so that the condensate cannot smoothly
transform into a single droplet. For the non-vortex case this regime has been studied in experiments and an array of droplets observed to form. An interesting question is how the presence of the vortex super-current will effect the dynamics of droplet formation in this case? E.g. will the droplets be observed to rotate after they form?
Bibliography


