CRITICAL VELOCITY AND
NUCLEATION OF DARK SOLUTIONS
IN NON-LOCAL NONLINEAR MEDIA

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DEDICATION

Dedicated to my mother and my sister, whose support made this journey possible.
Life is really simple, but we insist on making it complicated.

– Confucius
ABSTRACT OF THE THESIS

Critical Velocity And Nucleation Of Dark Solitons In Non-Local Nonlinear Media

by

Carlos Alberto Prieto Gómez

Master of Science with a Concentration in Dynamical Systems
San Diego State University, 2013

A Bose-Einstein condensate (BEC) is the state of matter of bosonic particles at ultra-cold temperatures. The Gross-Pitaevskii (GP) equation, a variant of the nonlinear Schrödinger equation (NLS) that includes an external trapping, is effectively described by the mean-field dynamical properties of BECs. Experimental progress has been possible to create BECs with particles with a strong dipolar moment, as in chromium, $^{52}$Cr. The dipole-dipole interaction adds a nonlocal term to the GP equation in the form of a convolution. Previous work has focused on vortex nucleation in non-dipolar condensates by dragging impurities through the condensate at supercritical speeds. For a one-dimensional GP equation with no external potential nor dipolar effects, a critical velocity can be found analytically above which dark (grey) solitons are emitted from the moving impurity. However, the case pertaining to the supercritical velocity for nucleation in dipolar condensates has yet to be considered. In this thesis, we present analytical approximations and numerical results for the critical velocity at which nucleation of dark solitons occurs in the one-dimensional dipolar GP equation.
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CHAPTER 1
INTRODUCTION

A Bose-Einstein condensate (BEC) is a state of matter consisting of a dilute atomic gas brought to ultra-cold temperatures near absolute zero. BECs can be modeled with the Gross-Pitaevskii (GP) equation, via mean-field approximations, assuming first-order, two-body contact interaction between atoms. In the presence of dipole-dipole interactions, BECs have long-range interactions between the particles, which introduces a new behavior regime that has sparked recent interest. This thesis focuses on a variant of the GP equation, where the dipole-dipole interaction is taken into consideration as a non-local effect described with a convolution term. Specifically, we focus on the effects of the dipolar interaction on the nucleation of dark solitons, and vortices in one- and two-dimensional condensates, respectively.

The GP equation we consider herein belongs to the family of nonlinear Schrödinger (NLS) equations. For bosonic particles, considering delta interactions between particles, the mean-field approximation gives rise to the nonlinear term in the NLS. The NLS can also describe additional phenomena like the evolution of water waves and the propagation of pulses in nonlinear optical fibers [21]. The nonlinearity in these equations allows for solitary waves known as solitons and vortices. This chapter discusses some of the background information on BECs and how vortices are generated. The three-dimensional dipolar GP equation is introduced in this chapter, and the model is reduced to a one-dimensional equation in Chapter 2.

1.1 BACKGROUND ON ULTRA COLD PHYSICS

Superfluidity, superconductivity, and Bose-Einstein condensation are phenomena that show surprising properties in the field of low-temperature quantum physics. While most quantum effects appear at the subatomic scale, superfluids and superconductors manifest quantum effects at larger scales, thus, usually referred to as macroscopic quantum phenomena. The phenomenon of Bose-Einstein condensation, as its name implies, was originally predicted by Bose and Einstein in 1924 [24]. In particular, it was shown that below a critical temperature, $T_c$, a finite fraction of particles of a Bose gas condenses into the same quantum state, transitioning into a state of matter known as the Bose-Einstein condensate.
BECs are recognized after the other four states of matter: solid, liquid, gas and plasma.

Unlike the superconductivity phenomenon, BECs were first predicted and then experimentally achieved 70 years later. The major difficulty in producing a BEC was to obtain temperatures close to absolute zero. This important achievement took place in 1995 and has already been recognized through the 2001 Nobel prize in Physics [16]. The temperature at which the first condensate was produced is below 170 nanokelvin (nK); this condition was achieved by combining laser and evaporating cooling techniques. Approximately two thousand Rubidium atoms, \(^{87}\text{Rb}\), achieved this critical temperature, creating the first condensate inside a magnetic field trap. Presently, hundreds of laboratories around the globe drive this field of research with experimental observations of condensates. Research is being developed in different magnetic trap (parabolic) and optical (periodic) configurations and with different kinds of particles, like sodium, lithium, hydrogen, chromium, and even photons [2, 8, 20, 37].

### 1.2 Basic Principles on Bose-Einstein Condensates

Bosons are particles with integer spin and, thus, can occupy the same quantum state, \(i.e.,\) they do not obey Pauli’s exclusion principle like fermions do. The condensation of the atoms is usually done under a harmonic potential

\[
V_{\text{ext}}(\vec{x}) = \frac{m}{2} \sum_{i=1}^{3} \Omega_i^2 x_i^2,
\]

where \(i\) corresponds to the different Cartesian dimensions and \(m\) is the mass of the atoms.

Each trap frequency, \(\Omega_i\), determines the characteristic harmonic oscillator length, \(a_i\), such that

\[
a_i^2 = \frac{\hbar}{m\Omega_i},
\]

where \(\hbar\) is the reduced Planck constant. The relative strength of the frequencies \(\Omega_i\) along the different directions determines the effective dimensionality of the problem. Namely, is \(\Omega_z \ll \Omega_x \approx \Omega_y\), the BEC is quasi-one dimensional and if \(\Omega_x \approx \Omega_y \ll \Omega_z\) the BEC is quasi-two dimensional.

At high temperatures, the Heisenberg principle dictates that particles are well localized. As temperature is reduced, the kinetic energy of the particles decreases, and following the uncertainty principle, the uncertainty of position increases. The wave nature of the particles becomes more apparent at low temperatures. These waves have an associated wavelength inversely proportional to the particle’s kinetic energy. The thermal de-Broglie
wavelength of a gas particle at temperature $T$ is given by:

$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}},$$

where $k_B$ is Boltzmann constant [62]. Once the critical temperature is reached, the individual wavelengths overlap, and all particles fall into the lowest quantum state [34]. Bose-Einstein condensation occurs when the thermal de-Broglie wavelength is in the same order of magnitude as the mean inter-particle spacing.

The mean inter-particle spacing is defined as $\langle r \rangle \propto \left(\frac{1}{n}\right)^{\frac{1}{3}}$, where $n$ is the particle density. If the phase-space density, $\varrho$, is defined as the product of particle density and the volume occupied by the wave function (de-Broglie wavelength cubed), $\varrho = n\lambda_{dB}^3$, then the transition is evident when $\varrho \approx 1$.

When the temperature reaches the critical value $T = T_c$, then $n = \frac{N}{\prod_{i=1}^{3} R_i}$ where $N$ is the number of atoms and the cloud size along each of the three dimensions are in the order of $R_i^2 \sim \frac{k_B T}{m \Omega_i^2}$. The relation of the transition temperature, the number of particles, and the geometric mean harmonic oscillator frequency, $\bar{\Omega} = \left(\prod_{i=1}^{3} \Omega_i\right)^{\frac{1}{3}}$, is then given by:

$$k_B T_c = C\hbar \bar{\Omega} N^{\frac{2}{3}}, \quad (1.2)$$

where $C$ is a constant that depends on the effective dimensionality of the BEC [51]. In the three-dimensional (3D) setting with a harmonic trap, the constant $C$ takes the value $C = \frac{1}{\zeta(3)^{\frac{2}{3}}} \approx 0.94$ where $\zeta(\alpha) = \sum_{n=1}^{\infty} n^{-\alpha}$ is the Riemann zeta function.

The transition temperature for lighter atoms is correspondingly higher, given that lighter elements have larger de-Broglie wavelength for an identical temperature. In order to achieved observations of BECs, atoms need large elastic collisional rates and low inelastic collisional rates to reach thermal equilibrium. The difficulty for experimentalist work in dipolar BECs is not the temperature, but the collisional properties of the atoms. Chromium has strong inelastic collisions, causing considerable mass loss of the condensate as the temperature is decreased. Physicists have already developed two techniques to lower the temperature of atom samples without significant mass loss: laser cooling and evaporative cooling. Finding the right geometry and trapping sequence, allows the BEC of Chromium to exist around $100 \text{nK}$ [15].
1.3 The Gross-Pitaevskii Equation

The basic physical model that describes the dynamical properties of the BEC is the GP equation. The GP equation describes the quantum state of the macroscopic wavefunction, \( \psi \). The GP equation, obtained by a mean-field approximation to the many-body Schrödinger equation of the interatomic contact interactions inside the condensate [7, 52] may be written as:

\[
i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}} \psi + g_{3D} |\psi|^2 \psi,
\]

where the complex function \( \psi(\vec{x}, t) \) is the wavefunction of the condensed atoms of mass \( m \). \( |\psi|^2 \) corresponds to the density of the condensate and \( \nabla^2 \) is the three-dimensional Laplacian operator. The nonlinear coefficient is defined as \( g_{3D} = \frac{4\pi \hbar^2 a_s}{m} \), where \( a_s \) is the s-scattering length that represents the contact interactions at the atomic level. When \( a_s \) is positive, the interaction between the atoms is repulsive; when \( a_s \) is negative, it is attractive. This is the key factor that most BECs are described as either ‘attractive’ or ‘repulsive’.

The GP equation can be derived by describing \( N \) particles of mass \( m \) trapped in an external potential \( V_{\text{ext}} \). The corresponding many-body Hamiltonian is

\[
\hat{H} = \int \hat{\Psi}^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) \right] \hat{\Psi}(r) \, dr
+ \frac{1}{2} \int \int \hat{\Psi}^\dagger(r) \hat{\Psi}^\dagger(r') U_{\text{int}}(r - r') \hat{\Psi}(r') \hat{\Psi}(r) \, dr \, dr',
\]

where \( V_{\text{int}} \) is the particle-particle interaction potential. \( \hat{\Psi}(r) \) and \( \hat{\Psi}^\dagger(r) \) are the boson field operators that represent the annihilation and creation of particles at position \( r \). The time evolution of the field operator is given by the Heisenberg equation:

\[
i\hbar \frac{\partial \hat{\Psi}(r, t)}{\partial t} = [\hat{\Psi}(r, t), \hat{H}],
\]

where \([A, B] = AB - BA\) denotes the commutator between two operators \( A \) and \( B \). Eq. (1.5) combined with Eq. (1.4) lead to the following expression:

\[
i\hbar \frac{\partial \hat{\Psi}(r, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + \int \hat{\Psi}^\dagger(r', t) U_{\text{int}}(r - r') \hat{\Psi}(r', t) \, dr' \right] \hat{\Psi}(r, t).
\]

The macroscopic occupation of the condensate can be expressed as:

\( \hat{\Psi}(r, t) = \psi(r, t) + \hat{\Psi}'(r, t) \) known as the Bogoliubov approximation [42]. \( \psi(r, t) = \langle \hat{\Psi} \rangle \) is the macroscopic wave-function of the condensate and \( \hat{\Psi}' \) describes the non-condensed particles. The mean field approximation consists of neglecting the quantum fluctuations \( \hat{\Psi}' \) when all particles are condensed below the critical temperature and thus

\[
i\hbar \frac{\partial \psi(r, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + \int \psi(r', t)^* U_{\text{int}}(r - r') \psi(r', t) \, dr' \right] \psi(r, t).
\]
Under the consideration of a weakly interacting dilute gas, the interactions can be considered short range. This approximation is good in the dilute-gas limit, where the inter-particle distance $n^{-\frac{1}{3}}$ is much larger than $s$-wave scattering length $a_s$. In such cases, the particle-particle interaction potential is effectively $U_{\text{int}}(r) = g_{3D} \delta(r)$, where $\delta(r)$ is the Dirac delta function and, as mentioned above, $g_{3D}$ is the constant proportional to $a_s$. Eq. (1.3) is a particular case of Eq. (1.7) when the interaction is a delta function which gives the cubic nonlinear characteristic to the GP equation.

The GP has two constants of motion. The total mass of the condensate

$$N = \int |\psi(\bar{x})|^2 \, d\bar{x},$$

(1.8)

and the total energy of the system

$$E = \int \frac{\hbar^2}{2m} |\nabla \psi(\bar{x})|^2 + V_{\text{ext}}|\psi(\bar{x})|^2 + \frac{g_{3D}}{2}|\psi(\bar{x})|^4 \, d\bar{x}.$$  

(1.9)

A subset of solutions known as ‘steady states’, $\psi_0$, have a constant density over time. Owing to the oscillatory behavior of the complex wavefunction, the real and imaginary part of $\psi_0$ return to the original position. The associated frequency for such oscillatory behavior is $\Upsilon = \frac{\mu_{3D}}{\hbar}$, where $\mu_{3D}$ is known as the chemical potential within the BEC context. A way to add the frequency term in the GP equation exists by doing a transformation $\psi \rightarrow \psi \exp[-i\frac{\mu_{3D}}{\hbar}t]$, which adds the linear term $-\mu_{3D}\psi$ in the right hand side of Eq. (1.3). This formulation is not used here, but the parameter $\mu_{3D}$ will play a special role later on. To find steady states of the GP equation, the separation of variables (time and space) $\psi(\bar{x}, t) = \psi_0(\bar{x}) \exp\left(-i\frac{\mu_{3D}}{\hbar}t\right)$ renders Eq. (1.3) to the time independent equation:

$$\mu_{3D}\psi_0 = -\frac{\hbar^2}{2m} \nabla^2 \psi_0 + V_{\text{ext}} \psi_0 + g_{3D} |\psi_0|^2 \psi_0.$$  

(1.10)

The GP is a variant of the famous NLS incorporating the external potential (or magnetic trap $V_{\text{ext}}$). A similar model is used in the study of wave propagation in fiber optics with a Kerr medium [35, 36]. In the optical setting, the light beam is assumed to propagate in the $r$ direction, and diffraction occurs in the transverse direction. The intensity of the light beam is represented by $|\psi|^2$. Nonlinearity arises from the dependence of the refraction index on the intensity of the propagating wave. In simple words, one can say that the media responds to the light propagating through it. A self-focusing medium corresponds to $g < 0$ and a self-defocusing medium to $g > 0$, and the general one-dimensional NLS is given by

$$i\frac{\partial \psi}{\partial z} = -\frac{1}{2} \partial_r^2 \psi + g|\psi|^2 \psi.$$  

(1.11)
1.4 Dipolar Condensates

The focus here is to consider one of the many other types of nonlinearity in the GP equation that are also possible. For instance, instead of considering two-body collisions as done previously, if one considers higher-order collisions, this leads to a cubic-quintic nonlinearity [11]. Also, in the optical models, the medium response displays saturation to the response of the propagating light giving rise to saturable-type nonlinearity [32, 56]. More complex models for the interaction potential consider the effects of short-range interactions (like two-body collisions) and long-range interactions, which in general bestow a nonlocal aspect to the GP equation. This thesis focuses on the interactions consisting of a local contact interaction and a long range dipole-dipole interaction potential: \( U_{\text{int}} = U_{\text{contact}} + U_{\text{dd}} \). The dipole-dipole interaction potential can be written as a function of \( \vec{r} \), the vector connecting the two particles, as:

\[
U_{\text{dd}}(\vec{r}) = \frac{C_{\text{dd}} \, \vec{e}_1 \cdot \vec{e}_2 - 3(\vec{e}_1 \cdot \hat{r})(\vec{e}_2 \cdot \hat{r})}{r^3}.
\]

(1.12)

Here, \( \vec{e}_i \) is the direction of the dipolar moment of the \( i \)-th particle, \( r = \|\vec{r}\| \), and \( \hat{r} \) is the unit vector in the direction of \( \vec{r} \) [30]. When particles have a magnetic dipole moment of magnitude \( d_m \), then \( C_{\text{dd}} = \mu_0 d_m^2 \), where \( \mu_0 \) is the permeability of vacuum. When particles have an electric moment of magnitude \( d_e \), then \( C_{\text{dd}} = \frac{d_e^2}{\epsilon_0} \), where \( \epsilon_0 \) is the permittivity of vacuum.

A polarized condensate has all the dipoles aligned the same dipolar direction, \( \vec{n} \). In such a case, equation Eq. (1.12) simplifies this to:

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

(1.13)

where \( \theta \) is the angle between the polarization direction, \( \vec{n} \), and the relative position of the particles, \( \vec{r} \). Given that this potential convolutes with the density, the effective potential is normally referred as a kernel function.

Dipole-dipole interactions have attracted recent interest because of the amount of experimental progress that has been vested to create BECs with polar particles such as chromium [6, 13, 14, 29]. The two most important properties of the dipole-dipole interaction are nonlocal, given the strength decays as \( \frac{1}{r^3} \), and the anisotropic interaction because the sign and strength of the interaction depend on the angle \( \theta \). The interaction potential \( U_{\text{dd}}(r) \propto \frac{1}{r^3} \) at long distances and plays a crucial role in the stability of solitary waves [19, 43]. As \( \theta \) varies between 0 and \( \pi/2 \), the numerator \( 1 - 3 \cos^2(\theta) \) varies between \(-2\) and \(1\). Thus the interaction can be either repulsive or attractive. The dipolar version of the GP equation may
now be written as:

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}} \psi + g_{3D}|\psi|^2 \psi + g_{dd} \left( \int \frac{1 - 3 \cos^2(\theta)}{|r - r'|^3} |\psi(r')|^2 \, dr' \right) \psi. \tag{1.14} \]

Here, \( g_{dd} = \alpha \frac{C_{dd}}{4\pi} \) is the nonlocal dipolar constant. Similar to how physicists are able to tune the scattering length through Feshbach resonances [38, 50], the dipole-dipole coupling can be tuned by a rotating polarization field [61], as shown in Figure 1.1. If the dipolar direction is rotated around the \( z \)-axis on a cone of aperture \( 2\varphi \), then the time average potential will have the factor \( \alpha = \frac{3 \cos^2(\varphi) - 1}{2} \). Thus, as \( 0 < \varphi < \frac{\pi}{2} \), then \( -\frac{1}{2} \leq \alpha \leq 1 \), which allows control of the dipolar strength to be either repulsive or attractive [27, 57]. The model described by Eq. (1.14) is the focus of this thesis.

Figure 1.1. The diagram for the variables for the interaction between two particles located at a relative distance, \( \vec{r} \) is represented by the dashed line. The dipolar moments, shown in solid (red) arrows, are rotated around the vertical \( z \)-axis on a cone of aperture \( 2\varphi \). The effective polarization direction is shown as the \( z \)-axis. The angle between the effective polarization direction and the distance between the two particles is \( \theta \).
1.5 Solitons and Vortices

The fundamental phenomena that appears in BECs and in general systems with the NLS model are localized and coherent structures [47]. In 1D, the NLS equation in particular has exact analytical solutions of nonlinear waves, which travel without changing form. Similar behavior is expected in the GP Eq. (1.3), given that the nonlinearity allows for the mathematical description of solitary waves (solitons) and vortices [22].

For attractive BECs, solitons exists with a localized maximum density peak, which decays to zero, known as bright solitons. For example, in the one-dimensional attractive NLS, the exact solution for a traveling wave of Eq. (1.11), with \( g = -1 \), has the form:

\[
\psi(r, t) = \eta \text{sech}(\eta(r - vt)) \exp(i(kr - \mu t)),
\]

where \( \mu \) is the frequency, \( v \) is the velocity and \( k \) is the soliton wavenumber. The soliton has a peak density of \( \eta^2 \) and it is directly related with the spatial width of the soliton \( \frac{1}{\eta} \). The velocity \( v = \frac{\partial \mu}{\partial k} \) is equal to the soliton’s wavenumber \( k \). The equality \( \mu = \frac{1}{2}(k^2 - \eta^2) \) is known as the dispersive relation, which states that bright solitons exists if \( 2\mu \leq k^2 \). Fixing the value for \( \mu \), the velocity becomes dependent on the amplitude of the wave.

The density of solitons or any background disturbance in the attractive model tends to increase to infinity within a small finite amount of time, and the kinetic energy counteracts this increase. In 2D and 3D, the condensate is exposed to ‘collapsing’ where the density increases very rapidly in a small region before exploding outwards, if the number of atoms exceeds a critical value [23, 58].

In the repulsive species of condensates, soliton nomenclature depends on the dimensionality of the condensate. In a three-dimensional repulsive condensate, solitons are generally quantized vortex rings. In the quasi-two dimensional approximation, there are quantized vortices and vortex stripes that have been experimentally stabilized. A lattice of vortices can be experimentally reproduced, called the vortex lattice. In the quasi-one dimensional repulsive BECs, the solitons are called dark/grey solitons depending on their velocity (dark for stationary and grey for moving).

In general, solitons in the repulsive BECs are characterized by having localized depletion of density, as well as a non-zero phase-shift. The wavefunction \( \psi \) in Eq. (1.11) can be described as \( \psi(r, t) = \sqrt{\rho(r, t)} \exp(i\phi(r, t)) \), where \( \rho \) is a function describing the density.
and the function $\phi$ is a periodic function that describes the angular phase. The phase change is defined as the change of the phase around the center of the soliton:

$$S = \Delta \phi \bigg|_{x \to -\infty}^{x \to \infty},$$

that is the change in the argument at the boundaries of the condensate. In the case of dark soliton, the phase-shift is $\pi$; and for grey solitons, it decreases towards zero as the velocity increases.

In the absence of an external trap, the density of BECs in a one-dimensional setting increases away from the center of the dark soliton converging to a nonzero constant-density background. The following is an example of a dark soliton for the one-dimensional case of the repulsive NLS, $g = 1$:

$$\psi(r,t) = \sqrt{\rho \tanh(\sqrt{\rho}(r - vt)) \exp(i(kr - \mu t))}, \quad \text{(1.16)}$$

where the dispersive relation is $\mu = \frac{1}{2}(k^2) + \rho$. Similarly to the case of bright soliton, the dark soliton satisfies: $v = k$. The soliton exist in a constant background density $|\psi|^2 = \rho$, which should be a stable homogeneous solution to the NLS [11]. Notice that the modulus square is constant, but the value at one boundary differs:

$$\psi(r \to +\infty, t = 0) = -\psi(r \to -\infty, t = 0) = \sqrt{\rho}. \quad \text{(1.17)}$$

In Figure 1.2, we can appreciate the real and imaginary part of a stationary dark soliton placed on a background of $\rho = 2$, after a few seconds. The real and imaginary part oscillate, but the modulus square remains the same.

A modulational instability analysis is normally used to determine the exponential growth of plane waves. Dark solitons/vortices are indeed more stable than their bright counter parts. The parameter region for which dark solitons in dipolar BECs exist can be determined by the modulational instability analysis.

A crucial parameter in the topic at hand is the healing length: $\xi = (8\pi N a_s)^{-\frac{1}{2}}$ determined by the distance at which the kinetic energy $\sim \frac{\hbar^2}{2m \xi^2}$ and the interaction energy $\sim \frac{4\pi \hbar^2 a_s N}{m}$ are balanced [18, 51, 53]. The healing length is the minimal spatial scale over which the function $\psi$ can vary; thus, dark solitons and vortices have spatial widths of $O(\xi)$. A dimensional reduction will require having the transverse harmonic oscillator length $a_r < \xi$, namely, the confinement in the transverse plane will reduce the dynamics to be either one- or
Figure 1.2. An example of a dark soliton of the one-dimensional NLS. The dashed (green) and the dash-dotted (red) line correspond to the real and imaginary part, respectively, of wave function $\psi$. The solid (blue) line corresponds to the modulus square of the density of the soliton. The dark soliton is located on a constant background of 2.

two-dimensional because there is no space in the transverse direction to allow for any excitations to develop.

Within the context of optics with nonlinear Kerr media, the refractive index can also be considered as a nonlocal interaction [39, 41]. The convolution term was often neglected, and simplified as a cubic term, as in Eq. (1.11). Research on nonlocal nonlinear media also considers convolution with the beam intensity [40], where a narrow localized wave can induce a nonlinear response in the surrounding regions. Results obtained here may prove useful in the optical context as well, given that dark solitons in dipolar BECs with repulsive long-range interaction behave like solitons in a self-defocusing nonlocal media.

Experimentalists working on BECs are able to generate bright solitons with quick changes of the scattering length via Feshbach resonances. For repulsive condensates, a lattice of vortices occurs by stirring the condensate by means of the external trap [52]. Several ways exist to nucleate a vortex, including passing a blue tuned laser barrier across the condensate. The approach discussed, herein, is to nucleate vortices by moving a Gaussian impurity [12, 55, 59] and consider the effect of the dipole-dipole interaction. The critical velocity is approximated by the numerical solution of a differential equation; a very similar approach to
the analysis performed on the non-dipolar GP model [31].

1.6 Layout

The main purpose of this thesis is to enhance understanding of the effects of the nonlocal coupling constants in a dipolar BEC. The regime of stable condensates with competitive nonlinearities will be studied in the one-dimensional case. The focus is the stability regime of the dipolar BEC and the effects of its parameters in the dark soliton in BECs with dipole-dipole interactions. Because nucleation depends on the velocity (as well as the shape) of the impurity in non-dipolar BECs, the study is conducted analytically with calculations of the critical velocity in the one-dimensional case of the GP equation and verified with numerical simulations.

In Chapter 2, the one-dimensional model for the effective one-dimensional dipolar GP equation is described. This is done by a dimensional reduction using a separation of variables, following the results from Ref. [9]. The conservation of mass and energy for the dipolar GP equation is also developed in Chapter 2. An approximation of the effective dipolar kernel is needed for numerical simulations, thus, the dipolar kernel appears more similar to the kernel described in Ref. [17]. In order to find homogeneous steady states where the dark solitons will be placed, the parameter regime of the nonlinearities is found from the modulational instability carried out Chap. 3. The Newton-Krylov method to find steady states is discussed in Chap. 4, as well as a pseudo-spectral time-split algorithm for time integration. For theoretical predictions, a linear approximation of the critical velocity is found in Chap. 5 for the dipolar GP equation in a co-moving reference frame.

The growth rates of linearly unstable planes waves over a constant background are calculated for a range of spatial frequencies, corroborating the first predictions in Chap. 3. The critical velocity is found through numerical simulations for a set of configurations. The numerical results for the critical velocity are good for large value of frequency of the harmonic trap in the transverse direction.
CHAPTER 2
THE 1D DIPOLAR GP MODEL

In this chapter, we discuss the dimensional reduction of the dipolar GP equation to one dimension. This reduces the dipolar kernel to a one-dimensional expression that slowly decays without a singularity at zero. The approximation used in this thesis is the same as in Ref. [17]. The anisotropic nature of the dipole-dipole interaction will be evident in the strength of the nonlinear constants and it is dependent only on the component of the dipole interaction on the longitudinal direction. The strength of the effective one-dimensional dipolar kernel is dependent on the transverse trapping strength of the external potential acting on the condensed atoms.

2.1 ADIMENSIONALIZATION

For the mathematical approach, the model is first transformed into a dimensionless version. The full dipolar GP equation is given by:

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{ext}} \psi + g_{3D} |\psi|^2 \psi + g_{dd} \left( \int \frac{1 - 3 \cos^2(\theta)}{|r - r'|^3} |\psi(r')|^2 \, dr' \right) \psi, \]

where

\[ V_{\text{ext}}(\vec{x}) = \frac{m}{2} \left( \Omega_x^2 x^2 + \Omega_y^2 y^2 + \Omega_z^2 z^2 \right), \]

and the integral of the density is the number of atoms \( \int |\psi|^2 \, d\vec{r} = N \), and the nonlinear coupling constants are

\[ g_{3D} = a_s \frac{4\pi \hbar^2}{m}, \quad g_{dd} = \alpha \frac{C_{dd}}{4\pi}. \]

The dipole-dipole interaction potential is described by the kernel, \( K_{3D} \). Let \( \theta \) be the angle such that \( ||\vec{r}|| \cos(\theta) = \hat{n} \cdot \vec{r} \) where \( \hat{n} \) is the unitary vector that corresponds to the dipolar direction. Then the dipolar kernel in 3D takes the form:

\[ K_{3D}(\vec{r}) = \frac{1 - 3 \cos^2(\theta)}{|r|^3}. \]

A rescaling of the four basic quantities of the condensate is conducted to achieve a more compact form of the dipolar GP equation. Each length is rescaled by the minimal harmonic oscillator length: \( a_0 = \min \{a_x, a_y, a_z\} \), which means: \( x = a_0 X, y = a_0 Y, \) and...
$z = a_0 Z$. We define $\Omega_0 = \max \{\Omega_x, \Omega_y, \Omega_z\}$, where $a_i^2 = \frac{\hbar}{m\Omega_i}$. The dimensionless quantity for time is given by $t = \frac{T}{\Omega_0}$. Energy is then rescaled by $\hbar\Omega_0$, and thus $V_{\text{ext}}(\vec{x}) = \hbar\Omega_0 V_{3D}(\vec{X})$, where

$$V_{3D}(\vec{X}) = \frac{1}{2} \left( \omega_X X^2 + \omega_Y Y^2 + \omega_Z Z^2 \right), \quad (2.5)$$

and $\omega_i = \Omega_i / \Omega_0$. We now rescale density by a constant $k$, $|\psi|^2 = k^2 |\hat{\psi}|^2$, therefore

$$\frac{\partial \psi}{\partial t} = k\Omega_0 \frac{\partial \hat{\psi}}{\partial T}, \quad \nabla^2 \psi = \frac{k m \Omega_0}{\hbar} \nabla^2 \hat{\psi}. \quad (2.6)$$

One should notice that the dipolar term should not add any power of the constant $a_0$ from the rescaling process to the overall equation, given that any rescaling of the dipolar kernel is compensated by the integral substitution. Therefore, from Eq. (2.1)

$$i \frac{\partial \hat{\psi}}{\partial T} = -\frac{1}{2} \nabla^2 \hat{\psi} + V_{3D} \hat{\psi} + \frac{g_{3D} k^2}{\hbar \Omega_0} |\hat{\psi}|^2 \hat{\psi} + \frac{g_{dd} k^2}{\hbar \Omega_0} \left( \int \frac{1 - 3 \cos^2(\theta)}{|R - R'|^3} |\hat{\psi}(R')|^2 dR' \right) \hat{\psi},$$

given that: $\int |\psi|^2 \, dr = N$, then $k^2 = \frac{N}{a_0^3}$ is such that $\int |\hat{\psi}|^2 \, dR = \frac{N}{a_0^3 k^2} = 1$.

Finally, the dimensionless form of the GP equation is obtained:

$$i \frac{\partial \hat{\psi}}{\partial T} = -\frac{1}{2} \nabla^2 \hat{\psi} + V_{3D} \hat{\psi} + g_1 |\hat{\psi}|^2 \hat{\psi} + g_2 \left[ K_{3D} * |\hat{\psi}|^2 \right] \hat{\psi}, \quad (2.7)$$

and it is normalized such that $\int |\hat{\psi}|^2 \, dR = 1$, where the dimensionless nonlinear constants are now:

$$g_1 = \frac{4\pi N}{a_0} \quad g_2 = \frac{\alpha}{4\pi \hbar^2 \alpha_0}, \quad (2.8)$$

and the integral is denoted as the convolution operator, that is

$$\left[ K_{3D} * |\hat{\psi}|^2 \right] = \int K_{3D}(r - r') |\hat{\psi}(r')|^2 \, dr'. \quad (2.9)$$

The focus of this thesis is the study of the vortex nucleation with competitive nonlinearities, that is $g_1 g_2 \leq 0$. The kernel in Eq. (2.4) still manifests a singularity at zero. Physically, the singularity is of no importance since the integral of a closed volume converges, but numerically we cannot calculate the dipole-dipole at zero. The following section is the dimension reduction using a separation of variables. The dipolar kernel is reduced to other forms in the quasi-1D approach. In this chapter, a particular set of kernels are used that do not share the singularity at zero nor the anisotropy of the full three-dimensional kernel, as previously mentioned.
2.2 Dimensionality Reduction

Here, we will reduce the three-dimensional dipolar GP model
\[ i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \nabla^2 \psi + V_{3D} \psi + g_1 |\psi|^2 \psi + g_2 \left( \int K_{3D}(r-r') |\psi(r')|^2 \, dr' \right) \psi, \] (2.10)
into a one-dimensional partial differential equation. Here, \( \psi \) is the wave-function for a three-dimensional condensate with nonlinearity constant \( g_1 \) and \( g_2 \). We assume that the condensate is enclosed in a harmonic trap, \( V_{3D} = \frac{1}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \). Consider a trap strength in two transverse directions larger than the trap strength in the longitudinal dimension: \( \omega_\perp \gg \omega_z \) such that \( a_\perp \ll \xi \). Other requirements for the mean-field reduction include \( g_1 \max(|\psi|^2) \ll \omega_\perp \) and \( \max(K_{3D}) \ll \omega_\perp \), so that the contact interaction and the dipole-dipole interaction do not excite transverse modes and the condensate is in the ground state along the transverse direction. We follow the same procedure as in Ref. [9].

Reducing the dipolar GP equation to a one-dimensional system, the dipolar kernel may take different approximate forms. One of the most surprising effects of the dipolar kernel is that it contains a contact interaction. The mathematical identity
\[ \frac{r^2 \delta_{ij} - 3x_i x_j}{r^5} = -\nabla_i \nabla_j \frac{1}{r} - \frac{4\pi}{3} \delta_{ij} \delta(\vec{r}), \]
where \( r = |\vec{r}| \), and \( x_i \) is the \( i \)-th Cartesian component of the direction \( \vec{r} \). The term \( \delta(\vec{r}) \) is the Dirac delta function, \( \nabla_i \) denotes the derivative with respect to the \( i \)-th coordinate, and \( \delta_{ij} \) is the Kronecker delta, which is quite useful in this case [4, 26]. The original kernel Eq. (2.4) can be rewritten as [49]:
\[ K_{3D}(\vec{r}) = \frac{1}{r^3} \left( 1 - \frac{3(\vec{r} \cdot \hat{n})^2}{|\vec{r}|^2} \right) \]
\[ = -\partial_{nn} \left( \frac{1}{|\vec{r}|} \right) - \frac{4\pi}{3} \delta(\vec{r}). \] (2.11)
The three components of the dipole direction are now written as \( \hat{n} = (n_x, n_y, n_z) \). The notation
\[ \partial_{nn} = n_x^2 \partial_{xx} + n_y^2 \partial_{yy} + n_z^2 \partial_{zz} + 2n_x n_y \partial_{xy} + 2n_x n_z \partial_{xz} + 2n_y n_z \partial_{yz} \]
is used for the second derivative along the dipole axis. Thus, the kernel includes a contact interaction, \( \delta(\vec{r}) \), and a simpler kernel is formed. We define the parameter (in dimensionless units) \( \epsilon_{dd} = \frac{4\pi g_2}{3g_1} \), as the ratio determining the strength of the dipolar interaction compared with the local interaction.
\[ i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \nabla^2 \psi + V_{3D} \psi + \beta_1 |\psi|^2 \psi + \beta_2 \left[ \int \partial_{nn} \left( \frac{1}{4\pi |r - r'|} \right) |\psi(r')|^2 \, dr' \right] \psi. \]  

(2.12)

Thus, the effective coupling constants are now:

\[ \beta_1 = g_1 (1 - \epsilon_{dd}) \]
\[ \beta_2 = -4\pi g_2 = -3g_1 \epsilon_{dd}. \]

In physical terms, $\epsilon_{dd} = \alpha \frac{C_{dd}}{3g_{3D}}$ and the effective scattering length would be

\[ \hat{a} = a_s (1 - \epsilon_{dd}). \]

The kernel of the convolution in Eq. (2.12), $U_{3D}(\vec{r}) = \frac{1}{4\pi |\vec{r}|}$, is just one of the many forms in which the three-dimensional interaction potential can be written.

We use separation of variables $\psi(\vec{x}, t) = \Pi(x, y, t) u(z, t)$ where the transverse function $\Pi$ satisfies the two-dimensional quantum harmonic oscillator equation:

\[ \frac{1}{2} \nabla^2 \Pi - \frac{1}{2} \omega_\perp^2 (x^2 + y^2) \Pi + \mu_\perp \Pi = 0. \]  

(2.13)

The transverse function is

\[ \Pi(x, y, t) = \varpi(x, y) \exp(-i\mu_\perp t) \]
\[ = \sqrt{\frac{\omega_\perp}{\pi}} \exp \left( -\frac{\omega_\perp (x^2 + y^2)}{2} \right) \exp(-i\omega_\perp t) \]  

(2.14)

which satisfies Eq. (2.13) with a frequency of $\mu_\perp = \omega_\perp$. Function $\Pi$ is normalized, $\iint |\Pi|^2 \, dx \, dy = \iint |\varpi|^2 \, dx \, dy = 1$, and the separation of variables requires the integration along the $xy$ plane. Thus, we separate variables in Eq. (2.12), yielding

\[ i \frac{\partial u}{\partial t} = -\frac{1}{2} \frac{\partial^2}{\partial z^2} u + V_{1D} u + \beta_1 \iint |\varpi|^4 \, dx \, dy |u|^2 \, u \]
\[ + \beta_2 \left[ \iint \oint \oint \partial_{nn} \left( \frac{1}{4\pi |r - r'|} \right) |u(z')|^2 |\varpi(x', y')|^2 \, dx' \, dy' \, dz' \right] |\varpi|^2 \, dx \, dy \, u, \]  

(2.15)

where the external trap in the longitudinal direction is reduced to be $V_{1D}(z) = \frac{1}{2} \omega_\perp^2 z^2$. Since

\[ \iint |\varpi|^4 \, dx \, dy = \frac{\omega_\perp}{2\pi}, \]

then $\beta_1 \frac{\omega_\perp}{2\pi}$ is the nonlinear constant associated with the cubic term of Eq. (2.15), thus the nonlinear constants change based on the strength of the transverse frequency of the harmonic potential. Now, the last term in Eq. (2.15) still holds a local effect. To show this the kernel needs to be rewritten, and the second derivative along the dipole direction must be expanded with the derivatives along the Cartesian coordinates. In fact, the kernel $U(\vec{r}) = \frac{1}{4\pi |\vec{r}|}$ is the solution to the Poisson equation, that is $-\nabla^2 U(\vec{r}) = \delta(\vec{r})$, where
the Laplacian operator is performed over the Cartesian space \( \mathbb{R}^3 \) [4, 48].

The convolution operator and the derivative operator can be arranged in any order
\[ \partial_x [f * g](x) = [\partial_x f * g](x) = [f * \partial_x g](x). \]
Also, if a function is symmetric with respect to \( x \) and \( y \), that is, \( f(x, y) = f(y, x) \) then it is trivial to prove that \( \partial_{xx} f(a, b) = \partial_{yy} f(b, a) \).

With these two basic ideas and the fact that \( U \) and \( \varpi \) are symmetric with respect to \( x \) and \( y \), then:
\[
\begin{align*}
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[ \partial_{xx} U(x-x', y-y', z-z') \right] |u(z')|^2 |\varpi(x', y')|^2 \, dx' \, dy' \, dz' \\
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[ \partial_{yy} U(y-y', x-x', z-z') \right] |u(z')|^2 |\varpi(x', y')|^2 \, dx' \, dy' \, dz'
\end{align*}
\]

This is better written as:
\[
\partial_{xx} (U * |u\varpi|^2) = \partial_{yy} (U * |u\varpi|^2).
\]

Since the convolution of two even functions is an even function and the derivative of an even function is an odd function, considering \(|u\varpi|^2\) to be even with respect to \( x \) and \( y \), as in most physical conditions, the integration along the \( x \) and \( y \) of the mixed derivatives \( \partial_{xy}, \partial_{yz}, \partial_{yz} \) is zero. Therefore,
\[
\beta_2 \left( \int \partial_{nn} [U * |u\varpi|^2] \varpi(x, y) \, dx \, dy \right) = 3g_1 \epsilon_{dd} \left[ 1 - \frac{n_z^2}{2} \frac{\omega_\perp}{2\pi} |u(z, t)|^2 + \frac{1}{2} \int \partial_{zz} (U * |u\varpi|^2) \varpi(x, y) \, dx \, dy \right].
\]

The dipolar equation can now be written as:
\[
i \frac{\partial u}{\partial t} = -\frac{1}{2} \frac{\partial^2}{\partial z^2} u + V_{1D} \psi + G_1 |u|^2 u + G_2 \left[ \int \partial_{zz} (U * |u\varpi|^2) \varpi(x, y) \, dx \, dy \right] u,
\]
where the constants are now
\[
G_1 = \beta_1 \frac{\omega_\perp}{2\pi} + 3g_1 \epsilon_{dd} \frac{1 - n_z^2}{2} \frac{\omega_\perp}{2\pi},
\]
\[
G_2 = 3g_1 \epsilon_{dd} \frac{1 - 3n_z^2}{2}.
\]

By using a substitution of variables
\[
\tilde{x} = x - x', \quad \tilde{x}' = x + x',
\]
one obtains that the dipolar term in Eq. (2.18) can be written as

\[
\iint \partial_{zz} (U * |u|) \omega(x, y)^2 \, dx \, dy = \partial_{zz} \int K_2(z - z') |u(z')|^2 \, dz' = \partial_{zz} \left[ K_2 * |u|^2 \right],
\]

(2.21)

where

\[
K_2(z - z') = \iint \frac{\omega_\perp \exp(-\frac{\omega_\perp}{2} (\tilde{x}^2 + \tilde{y}^2))}{8\pi^2 \sqrt{\tilde{x}^2 + \tilde{y}^2 + (z - z')^2}} \, d\tilde{x} \, d\tilde{y}.
\]

(2.22)

Through the variable substitution

\[
\tilde{x} = r \cos(\theta),
\]

\[
\tilde{y} = r \sin(\theta)
\]

and the substitution of \(\xi^2 = \tilde{r}^2 + (z - z')^2\), the kernel at \(z - z'\) is in fact

\[
K_2(z - z') = \frac{\omega_\perp}{4\sqrt{2}\pi} \exp\left(\frac{\omega_\perp}{2} (z - z')^2\right) \left[ \sqrt{\frac{2\omega_\perp}{\pi}} \int_0^\infty \exp\left(-\frac{\omega_\perp}{2} \xi^2\right) d\xi \right].
\]

(2.24)

The term enclosed in brackets is a well-known integral, the complementary error function:

\[
\frac{2}{\sqrt{\pi}} \int_0^\infty \exp\left(-\frac{\omega_\perp}{2} \xi^2\right) \sqrt{\frac{\omega_\perp}{2}} d\xi = \text{erfc}\left(\sqrt{\frac{\omega_\perp}{2}} \right).
\]

(2.25)

A closed form for the dipolar term is much preferred in this thesis. The effective kernel that interacts with \(|u|^2\) through the convolution operator should be proportional to the second derivative of \(K_2\), that is, \(\partial_{zz} K_2 * |u|^2\). The second derivative of \(K_2\) has a closed form using the derivative of the complementary error function.

The model for a cigar-shaped dipolar BEC is:

\[
i \frac{\partial u}{\partial t} = -\frac{1}{2} \partial_{zz} u + V_{1D} u + G_1 |u|^2 u + G_2 \left[ K_{1D} * |u|^2 \right] u,
\]

(2.26)

where the nonlinear constants are:

\[
G_1 = \frac{g_1 \omega_r}{2\pi} \left[ 1 + \frac{\epsilon_{dd}(1 - 3n_z^2)}{2} \right],
\]

\[
G_2 = \frac{3g_1 \epsilon_{dd} \sqrt{\omega_r}}{8\sqrt{2}\pi} \left( 1 - 3n_z^2 \right) = \frac{4\pi g_2 \sqrt{\omega_r}}{8\sqrt{2}\pi} \left( 1 - 3n_z^2 \right).
\]

(2.27)

and the effective one-dimensional long range kernel of Eq. (2.18) has the closed form:

\[
K_{1D}(z) = \frac{\partial}{\partial z^2} \left[ \exp\left(\frac{\omega_\perp}{2} z^2\right) \text{erfc}\left(\sqrt{\frac{\omega_\perp}{2}} |z| \right) \right]
\]

\[
= \omega_r \left[ (1 + \omega_r z^2) \exp\left(\frac{\omega_r}{2} z^2\right) \text{erfc}\left(\sqrt{\frac{\omega_r}{2}} |z| \right) - \frac{2\omega_\perp}{\sqrt{\pi}} |z| \right].
\]

(2.28)
2.2.1 Conservation of Mass and Energy

The dipolar GP equation still poses two important constants of motion. We will also study the dynamics of the independent terms of energy. In the following subsection, the constants of motion for the one-dimensional dipolar GP are deduced. We assume that the flux at the boundary is zero.

Starting from the quasi-1D equation and its complex conjugate
\[
\begin{align*}
\frac{i}{2} \frac{\partial}{\partial t} u + \frac{1}{2} \nabla^2 u - V_{1D} u - g_1 |u|^2 u - g_2 [K_{1D} \ast |u|^2] u &= 0, \\
-\frac{i}{2} \frac{\partial}{\partial t} \overline{u} + \frac{1}{2} \nabla^2 \overline{u} - V_{1D} \overline{u} - g_1 |\overline{u}|^2 \overline{u} - g_2 [K_{1D} \ast |\overline{u}|^2] \overline{u} &= 0,
\end{align*}
\]
(2.29)
multiply each by \(\overline{u}\) and \(u\), respectively; subtract the two resulting equations to yield
\[
\begin{align*}
\frac{i}{2} \left( \frac{\partial u}{\partial t} u + \frac{\partial \overline{u}}{\partial t} \overline{u} \right) + \frac{1}{2} \left( \nabla^2 u - \nabla^2 \overline{u} \right) = 0,
\end{align*}
\]
(2.30)
\[
\Rightarrow \frac{i}{2} \frac{\partial}{\partial t} (u \overline{u}) + \frac{\partial}{\partial z} (u \overline{u} - \overline{u} u) = 0.
\]
Integrating with respect to \(z\) on \(-\infty < z < \infty\) gives that \(i \frac{\partial}{\partial t} (\int_{-\infty}^{\infty} |u|^2 dz) = 0\), conservation of mass, because the second term in Eq. (2.30) becomes zero since \(\lim_{z \to \pm \infty} \frac{\partial}{\partial z} (u \overline{u} - \overline{u} u) = 0\).

On the other hand, taking Eq. (2.29), multiplied by \(\overline{u}_t\) and \(u_t\) respectively, and adding the result yields
\[
\begin{align*}
&\frac{1}{2} \frac{\partial}{\partial z} (\overline{u}_t u_z + u_t \overline{u}_z) - \frac{1}{2} \frac{\partial}{\partial t} (u_z \overline{u}) - V_{1D} \frac{\partial}{\partial t} (|u|^2) \\
&- g_1 \frac{\partial}{\partial t} (|u|^4) - g_2 [K_{1D} \ast |u|^2] (u_t \overline{u} + \overline{u} u_t) = 0.
\end{align*}
\]
Integrating with respect to \(z\) on \(-\infty < z < \infty\) gives that
\[
\frac{\partial}{\partial t} (\int_{-\infty}^{\infty} -\frac{1}{2} |u_z|^2 - V_{1D} |u|^2 - \frac{g_1}{2} |u|^4 - \frac{g_2}{2} [K_{1D} \ast |u|^2] |u|^2 dz) = 0.
\]
The previous equation proves the conservation of energy, where the terms represent the kinetic, potential, (local) interaction, and (long-range) interaction energy, respectively. Using integration by parts and the fact that the flow is zero at the boundary, allows for easier calculation of the energy, by replacing \(\int_{-\infty}^{\infty} -\frac{1}{2} |u_z|^2 dz\) by \(\int_{-\infty}^{\infty} \frac{1}{2} \overline{u} \nabla^2 u dz\).

2.3 Approximation of the Dipolar Kernel

The closed form of the effective one-dimensional dipolar kernel, Eq. (2.28), obtained has a particular issue. Most numerical programs have limitations to calculate \(\exp(z^2)\) for large
values of $z$, even though the overall behavior is a decay towards zero, by the complementary error function, $\text{erfc}(|z|)$. An approximation proportional to the one used in Ref. [17] is used in this thesis.

The approximation for the one-dimensional kernel is:

$$K_1(z) = \omega_\perp k^3 \left( \frac{z^2 \omega_\perp}{2} + k^2 \right)^{-\frac{3}{2}},$$

(2.31)

where $k$ is a constant that permits that the integrals of the kernels to match. Function $K_1$ has a decay similar to $\frac{1}{z}$ for large $z$ values. Even though the similarities of the two dipolar kernels are not obvious, these share similar behavior in the Fourier space.

The value for the $k = \frac{1}{\sqrt{\pi}}$ allows

$$\int K_1(z) \, dz = \int K_{1D}(z) \, dz,$$

which is an important characteristic to be preserved. As the strength of the transverse frequency $\omega_\perp$ increases, the two dipolar kernels can be approximated by $\omega_\perp \delta(z)$. The two kernels are shown in Figure 2.1 for $\omega_\perp = 2$, the value chosen of Ref. [17].

![Figure 2.1. The effective 1D dipole-dipole interaction potentials for $\omega_\perp = 2$. The dash-doted (red) line corresponds to $K_{1D}$, and the solid (blue) line corresponds to $K_1$.](image-url)
The approximation allows us to bypass most of the difficulties calculating integrals such as:
\[
\int_{-\infty}^{\infty} K_1(z) \, dz = \lim_{L \to \infty} \frac{2\sqrt{2\omega_r}^{3/2} \sqrt{\frac{2+L^2\omega_r \pi}{\omega_r}} L}{2 + L^2 \omega_r \pi} = \frac{2\sqrt{2\omega_r}}{\sqrt{\pi}} \approx 1.595769 \sqrt{\omega_r}.
\]

We will also need to work with the Fourier transform of the effective dipolar kernel. At zero, the Fourier transform is reduced to the integral of the integrand \( K_1 \). The following expression is found through Maple and is valid for \( \hat{k} \neq 0 \)
\[
\mathcal{K}(\hat{k}) = \int K_1(z) \exp(-2\pi i \hat{k} z) \, dz = -2\pi \hat{k}i \left( Y \left( 1, 2\sqrt{2\pi i} \hat{k} \right) - Y \left( 1, -2\sqrt{2\pi i} \hat{k} \right) \right),
\]
where \( Y(\alpha, x) \) is the Bessel function of the second kind of order \( \alpha \). The Bessel functions of the second kind are characterized by having a singularity at zero, and having a oscillatory behavior towards zero. The Bessel functions are still valid for complex values. We write the Bessel function of the second kind as a combination of the modified Bessel functions.
\[
Y(\alpha, iz) = e^{\frac{(\alpha+1)\pi}{2}} I(\alpha, z) - \frac{2}{\pi} e^{-\frac{\alpha\pi}{2}} K(\alpha, z),
\]
which is valid since \( -\pi < \arg(z) \leq \frac{\pi}{2} \). \( K(\alpha, z) \) is known to have exponentially decaying behavior, and \( I(\alpha, z) \) to be exponentially increasing \([1]\). We can further simplify the Fourier transform by using the series equivalent of the modified Bessel functions. In particular, \( I(1, z) \) is an even function; \( K(1, z) \) is an odd function. Thus,
\[
\mathcal{K}(\hat{k}) = \begin{cases} 
\frac{2\sqrt{2\omega_r}}{\sqrt{\pi}} & \hat{k} = 0, \\
8|\hat{k}|K(1, 2\sqrt{2\pi} |\hat{k}|) & \hat{k} \neq 0.
\end{cases}
\]

Given that kernel \( K_1 \) is a real even function, its Fourier transform should also be an even real function. An example of the Fourier transform of the dipolar kernel, \( K_1 \) is shown in Figure 2.2.

### 2.4 The Moving Impurity

In order to nucleate dark solitons, an impurity in the external potential is set into motion at the center of the condensate. The impurity used here has the form of a velocity dependent Gaussian with a fixed standard deviation of \( \sigma = \sqrt{0.09} \), which is used in Ref. \([12]\). If the impurity moves at velocity \( \nu \), the external potential for the system reads:
\[
V_{ID}(z, t) = V_{har}(z) + V_{imp}(z, t),
\]
(2.35a)
Figure 2.2. The curve corresponds to the Fourier Transform of kernel $K_1$ for $\omega = 2$.

where

$$V_{\text{har}}(z, t) = \frac{1}{2}(\omega^2 z^2)$$

$$V_{\text{imp}}(z, t) = A \exp \left( -\frac{(z - \nu t)^2}{2\sigma^2} \right).$$

(2.35b)

Here, $A$ is the amplitude of the impurity. If the strength of the impurity is:

$$\int V_{\text{imp}}(z, t) \, dz = \beta,$$

then $A = \frac{\beta}{\sqrt{2\pi}\sigma}$.

It is very important for us that the motion of the impurity is made carefully. At the start of a numerical simulation, the impurity is located at $z = 0$. The velocity of the impurity increases adiabatically. Otherwise, the impurity starts by moving at a high velocity, and may generate unwanted localized excitations [3], adding the energy of the system; thereby, analysis of the energy would be unreliable.

Here, the velocity is increased slowly following parametrization by translation of a hyperbolic tangent. This function is usually used in many physical processes because it allows us to easily parametrize the transition from one state into another. We hoped for the velocity to be zero at the beginning; to start moving around a given time, $T_0$, but reached the velocity $\nu$ after a short time interval. The velocity at a time $t$, the velocity is given by.

$$v(t) = \nu \frac{1 + \tanh(2\kappa(t - T_0))}{2},$$

where $T_0$ is large. The parameter $\kappa$, determines the rate of change that occurs at $T_0$. At $t = T_0$, the velocity has reached half of the desired velocity, $\nu$, and for higher values of $\kappa$, the change occurs in a short time span. Even at small values of $\kappa$, in a time interval of $\frac{4}{\kappa}$ around the time the impurity starts its motion, the velocity changes from 0 to $\nu$. We show an example
of this transition in Fig. 2.3.

Figure 2.3. The velocity of the impurity increases slowly following the solid (blue) line. Here, the velocity increases from 0 to $\nu = 1$ around $T_0 = 10$. In this case, $\varkappa = 2$, and the vertical lines correspond to $T_0 \pm \frac{2}{\varkappa}$, to show that the transition has occurred in an interval of $\frac{4}{\varkappa}$.
CHAPTER 3
MODULATIONAL INSTABILITY FOR HOMOGENEOUS STATES

Bright solitons in the NLS are unstable in 2D and 3D. Modulational Instability (MI) analysis of the one-dimensional NLS, shows that for \( g_1 < 0 \), steady states of constant background are unstable. For the dipolar model, the nonlinearities may allow for the existence of complex perturbations of the homogeneous steady state to grow exponentially. With the reduced one-dimensional dipolar GP equation at hand, we study the linear MI of the constant background in the absence of an external potential. The exponential growth of the perturbation modes, or MI gain, is proportional to the background density, and thus, for high densities MI may appear for perturbations with small wave-number.

The parameter region of the nonlinear constants for which constant backgrounds are modulationally stable are found for a constant background of density 1. The approach taken here is to find the Bogoliubov-de Gennes equations in Fourier space so that the dipolar convolution may be more tractable. This allows for much better control of the operators and the convolution term that comes from the dipole-dipole interaction. The result is a relation of the exponential growth rates to the parameters of a dipolar NLS equation with a general long-range interaction. We construct the parameter space, \((g_1, g_2)\) of the nonlinearity constants, from the results obtained here.

3.1 Modulational Gain for the Dipolar GP Equation

From Chapter 2, the one-dimensional dipolar GP equation can be written as:

\[
i \frac{\partial \psi}{\partial t} + \frac{1}{2} \frac{\partial^2 \psi}{\partial z^2} - V_{1D} \psi - g_1 |\psi|^2 \psi - g_2 \int K_1(z - z') |\psi(z')|^2 \, dz' \psi = 0.
\]

In order to find a steady state, a simple transformation of the form \( \psi(z, t) = u(z)e^{-i\mu t} \), where \( u(z) \) is time independent, is replaced into Eq. (3.1), the following equation is obtained:

\[
\mu u + \frac{1}{2} \frac{\partial^2 u}{\partial z^2} - V_{1D} u - g_1 |u|^2 u - g_2 [K_1 * |\psi|^2] \psi = 0
\]

Eq. (3.2) can be solved numerically with a Newton algorithm to find steady states, if the chemical potential or frequency \( \mu \) is given. In this chapter, modulational instability
analysis is performed to find a parameter range where the homogeneous steady state is stable. Consider now a homogeneous state \( u(z) = u_0 \) in the absence of external potential \((V_{1D} \equiv 0)\). This yields

\[
\mu = \left( g_1 + g_2 \int K_1(z') \, dz' \right) |u_0|^2.
\] (3.3)

It may not appear obvious, but the constant

\[
G = g_1 + g_2 \int K_1(z') \, dz',
\]

will appear several times throughout this thesis, in particular, in the later chapters. This will become the effective nonlinearity constant.

Perturbation analysis can be done around a steady state \( u \) considering

\[
\psi = [u + \epsilon(ae^{\lambda t} + be^{-\lambda t})]e^{-i\mu t} = (u + \epsilon v)e^{-i\mu t},
\] (3.4)

where we denote \( v = ae^{\lambda t} + be^{-\lambda t} \) as the perturbation term, where \( a \) and \( b \) are complex functions that depend on the space variable \( z \). A linear perturbation with \( \Re(\lambda) > 0 \) implies the system is unstable. Both \( u \) and \( v \) have the same frequency \( \mu \), so that perturbation part \( v \) rotates at the same rate as the steady state \( u \).

The local and nonlocal terms can be expanded as:

\[
|u + \epsilon v|^2(u + \epsilon v) = |u|^2 u + \epsilon(u^2 \overline{v} + 2|u|^2 v) + O(\epsilon^2),
\]

and

\[
[K_1 * |u + \epsilon v|^2](u + \epsilon v) = [K_1 * |u|^2] (u) + \epsilon \left( [K_1 * (u \overline{v} + v \overline{u})] (u) + [K_1 * |u|^2] (v) \right) + O(\epsilon^2).
\]

We consider the notation:

\[
Z = \int K_1(z - z')|u(z')|^2 \, dz' = [K_1 * |u|^2],
\]

\[
K = [K_1 * (u \overline{v} + v \overline{u})] (u) + [K_1 * |u|^2] (v).
\]

We substitute the expansion for \( \psi \) given in Eq. (3.4) into Eq. (3.1) and collect together terms of the same order. The coefficients of each power of \( \epsilon \) on the two sides of the equation are compared; thus, the first two coefficients are equal to zero.

\[
O(\epsilon^0) : \quad \mu u + \frac{1}{2} \nabla^2 u - V_{1D} u - g_1 |u|^2 u - g_2 Z u = 0,
\]

\[
O(\epsilon^1) : \quad i\dot{v} + \mu v + \frac{1}{2} \nabla^2 v - V_{1D} v - g_1 (u^2 \overline{v} + 2|u|^2 v) - g_2 K = 0;
\] (3.5)
where it is clear that the first equation represents the time-independent dipolar GP equation. The linear perturbation term $K$ can be written in an easier form when: $v = ae^{\lambda t} + be^{\bar{\lambda}t}$. Defining the bilinear operator:

$$K(a, b) \equiv \int K_1(z - z')[u(z')\bar{b}(z') + a(z')\bar{u}(z')] dz'$$

$$\equiv K_1 \ast (u\bar{b} + a\bar{u}),$$

the dipolar term on the first-order perturbation can now be written as:

$$g_2K = e^{\lambda t} [g_2K(a, \bar{b})u + g_2Za] + e^{\bar{\lambda}t} [g_2K(b, \bar{a})u + g_2Zb].$$

Notice that $K(b, \bar{a}) = K(a, \bar{b})$ and $Z = Z$, given that the integration takes place over a real space with a real value $K_1$. Now, the second equation of Eq. (3.5) can be rewritten as

$$e^{\lambda t}(i\lambda a + \mu a + \frac{1}{2}\nabla^2a - g_1[u^2b + 2|u|^2a] - g_2K(a, \bar{b})u - g_2Za - V_{1D}a) = 0,$$

$$e^{\bar{\lambda}t}(i\bar{\lambda}b + \mu b + \frac{1}{2}\nabla^2b - g_1[u^2\bar{a} + 2|u|^2\bar{b}] - g_2K(b, \bar{a})u - g_2Zb - V_{1D}b) = 0. \quad (3.6)$$

Therefore, these two equations have the following invariants:

1. $\lambda \leftrightarrow \bar{\lambda}$ and $a \leftrightarrow b$, the equations will be unchanged.
2. $\lambda \leftrightarrow -\bar{\lambda}$, $a \leftrightarrow \bar{a}$, and $b \leftrightarrow \bar{b}$, the equations are now their complex conjugates.

Consequently, if $\lambda$ is an eigenvalue, so is $\bar{\lambda}$, and $-\bar{\lambda}$. It is clear that by following the same idea for $\bar{\lambda}$, $-\lambda$ would also be an eigenvalue, and thus the eigenvalues appear in quartets.

Finally a linearized system for the perturbation eigenmodes can be written as

$$\lambda \begin{pmatrix} a \\ b \end{pmatrix} = iM_1 \begin{pmatrix} a \\ b \end{pmatrix},$$

where $M_1$ is the matrix of operators:

$$M_1 = \begin{bmatrix} \mu + \frac{1}{2}\nabla^2 - 2|u|^2 - V_{1D} & -g_1u^2 \\ g_1\bar{u}^2 & -\mu - \frac{1}{2}\nabla^2 + 2|u|^2 + V_{1D} \end{bmatrix} - 2|u|^2 - V_{1D} + g_2u[K_1 \ast \bar{u}],$$

$$g_2u[K_1 \ast \bar{u}] + g_2Z + g_2\bar{u}[K_1 \ast \bar{b}u].$$

This can be written as: $M_1 = \begin{bmatrix} L_1 & L_2 \\ -L_2 & -L_1 \end{bmatrix}$ where

$$L_1 = \mu + \frac{1}{2}\nabla^2 - 2|u|^2 - V_{1D} - g_2Z - g_2u[K_1 \ast \bar{u}],$$

$$L_2 = -g_1u^2 - g_2u[K_1 \ast u]. \quad (3.7)$$
Applying the steady state $\psi_s = u_0 e^{-i\mu t}$ of constant background, where 
$\mu = |u_0|^2 (g_1 + g_2 \int K_1(z') dz')$, yields

$$\mu a - 2g_1 |u_0|^2 a - g_2 Z a = -g_1 |u_0|^2 a,$$

where $Z = [K_1 * |u_0|^2] = |u_0|^2 \int K_1(z') dz'$.

Therefore, Eq. (3.6) can be expressed as

$$\lambda a = i \frac{1}{2} \nabla^2 a - g_1 u_0^2 (a + \bar{b}) - g_2 K(a, \bar{b}) u_0],$$

$$\lambda \bar{b} = -i \frac{1}{2} \nabla^2 \bar{b} - g_1 u_0^2 (\bar{b} + a) - g_2 K(b, \bar{a}) \bar{u}_0].$$

(3.8)

Notice that for $u_0$ real:

$$K(a, \bar{b}) u_0 = u_0^2 \int K_1(z - z')(a(z') + \bar{b}(z')) dz',$$

$$K(b, \bar{a}) \bar{u}_0 = K(a, b) u_0.$$

Eq. (3.8) is hard to handle with the convolution term, thus, in this case a Fourier transform is performed in the system obtained, and the linear system allows for better control of the perturbation parameter functions $a$ and $b$. Defining $A$ and $B$ as the Fourier transform of the functions $a$ and $b$, respectively, will consider each function as a combination of plane wave with wave-number $2\pi \hat{k}$. Also, $\mathcal{K}$ is defined as the transform of the real symmetric function $K_1$. For the dipolar case, the analysis will be based on the following properties of the Fourier transform:

$$A(\hat{k}) = \mathfrak{F}_a(a(z))(\hat{k}) = \int a(z) \exp(-2\pi i \hat{k} z) dz,$$

$$B(-\hat{k}) = \mathfrak{F}_b(b(z))(\hat{k}) = \int \bar{b}(z) \exp(-2\pi i \hat{k} z) dz,$$

$$B(-\hat{k}) = B(\hat{k}) \text{ if } b \text{ was a real function},$$

$$\mathfrak{F}[K_1 * u](\hat{k}) = \mathcal{K}(\hat{k}) \cdot \mathfrak{F}[u(z)](\hat{k})$$

$$\mathfrak{F}[(\nabla^2 u(z))(\hat{k})] = (2\pi i \hat{k})^2 \mathfrak{F}[u(z)](\hat{k}).$$

Using those properties, one may transform Eq. (3.8) into:

$$M \begin{pmatrix} A \\ B \end{pmatrix} = \bar{0},$$

(3.9)

where

$$M = \begin{bmatrix}
-2\pi^2 \hat{k}^2 - g_1 u_0^2 - g_2 u_0^2 \mathcal{K} + i \lambda & -g_1 u_0^2 - g_2 u_0^2 \mathcal{K} \\
-g_1 u_0^2 - g_2 u_0^2 \mathcal{K} & -2\pi^2 \hat{k}^2 - g_1 u_0^2 - g_2 u_0^2 \mathcal{K} - i \lambda
\end{bmatrix}.$$
A nontrivial solution is possible if \( \det(M) = 0 \)

\[
\det(M) = (-2\pi^2 \hat{k}^2 - g_1 u_0^2 - g_2 u_0^2 \mathcal{X} + i\lambda)(-2\pi^2 \hat{k}^2 - g_1 u_0^2 - g_2 u_0^2 \mathcal{X} - i\lambda)
- (-g_1 u_0^2 - g_2 u_0^2 \mathcal{X})^2
\]

\[
= (2\pi^2 \hat{k}^2 + g_1 u_0^2 + g_2 u_0^2 \mathcal{X})^2 + \lambda^2 - (g_1 u_0^2 + g_2 u_0^2 \mathcal{X})^2 = 4\pi^4 \hat{k}^4 + 2(2\pi^2 \hat{k}^2)(g_1 u_0^2 + g_2 u_0^2 \mathcal{X}) + \lambda^2 = 0,
\]

which yields

\[
\lambda^2 = -4\pi^2 \hat{k}^2 (\pi^2 \hat{k}^2 + (g_1 u_0^2 + g_2 u_0^2 \mathcal{X})).
\]

Notice that \( \lambda \) is purely imaginary, and, therefore, without instability, when \( \pi^2 \hat{k}^2 + u_0^2(g_1 + g_2 \mathcal{X}(\hat{k})) > 0 \). Modulational instability can occur for small values of \( \hat{k} \). In the purely attractive case, where \( g_1 \) and \( g_2 \) have both negative values, modulational instability is found even at \( \hat{k} = 0 \) since \( g_1 + g_2 \mathcal{X}(0) = g_1 + g_2 \int K_1(z) \, dz < 0 \).

The modulational instability gain is defined as the positive real part of the eigenvalue, \( \Lambda = \Re(\lambda) \):

\[
\Lambda(\hat{k}) = 2\pi \left| \hat{k} u_0 \right| \Re \left( \sqrt{-\left( g_1 + g_2 \mathcal{X}(\hat{k}) \right) - \frac{\pi^2 \hat{k}^2}{u_0^2}} \right)
\]

(3.13)

**3.2 Analysis of the Modulational Gain**

The previous function, \( \Lambda(\hat{k}) \) corroborates the idea that homogeneous backgrounds are unstable in the case of attractive BECs, and modulatorally stable for repulsive BECs. We can clearly see that there is no modulational gain for repulsive BEC for a large wave-number region and large densities in Figure 3.1, and there is modulational gain for small wave-numbers for the attractive BEC, as seen in Figure 3.2.

To support dark solitons, they must be planted on modulatorally stable constant backgrounds. For BEC with no dipole-dipole interaction, \( g_2 = 0 \), one may find that dark solitons are only possible with \( g_1 > 0 \). In such cases, the frequency is also positive: \( \mu > 0 \). As a preliminary result, one may notice the limitations of the parameter range: \( g_1 + g_2 \int K_1(z) \, dz > 0 \), where the effective nonlinearity is positive. This implies that the allowable region of the plane \( (g_1, g_2) \) for dark solitons is located above the line given by

\[
y = -x \left( \int K_1(z) \, dz \right).
\]

The modulational instability gain function is proportional to the absolute value of the wavenumber, \( |\hat{k}| \) and the constant background \( |u_0| \). We can simplify the idea of instability and
The modulational gain is shown for \( g_2 = 0 \), and \( g_1 = 1 \), which is a repulsive GP system. Background density takes values between 1 and 10, and wave number from \(-10\) to 10.

Figure 3.1. The modulational gain is shown for \( g_2 = 0 \), and \( g_1 = 1 \), which is a repulsive GP system. Background density takes values between 1 and 10, and wave number from \(-10\) to 10.

declare that modulational instability occurs when

\[
H(\hat{k}, g_1, g_2, u_0) = g_1 + g_2 \mathcal{K}(\hat{k}) + \left(\frac{\pi \hat{k}}{u_0}\right)^2 < 0, \tag{3.14}
\]

where \( \mathcal{K} \) is the Fourier transform of the kernel in the nonlocal interaction term of the dipolar GP. The Fourier transform of the dipolar kernel is known as

\[
|\hat{k}| \mathcal{K}(1, 2 \sqrt{\frac{2\pi}{\omega_\perp}} |\hat{k}|) \text{ for } \hat{k} \neq 0.
\]

Therefore the Fourier transform resembles a concave parabola at the height given by \( \int K_1(z') dz' \), such that \( \hat{k} \gg 20 \frac{\sqrt{\omega_\perp}}{2\sqrt{2}} \), the Fourier transform is close to zero. Thus, the \( g_1 + g_2 \mathcal{K}(\hat{k}) \) in the modulational gain function is a translation of such bell shape function, where \( g_2 \) and \( g_1 \) control the height and vertical translation of the bell shape respectively. The background density \( u_0 \) controls the width of the parabola given by the factor \( \left(\frac{\pi \hat{k}}{u_0}\right)^2 \).

In the case of nonlocal interaction, the modulational gain for fixed value of \( g_1 \) and \( g_2 \), for \( \omega_\perp = 2 \) for a range of densities and wavenumbers are shown in Figures 3.3 and 3.4. As mentioned before \( g_1 + g_2 \int K_1(z') dz' < 0 \) is unstable for small wavenumber values. For \( g_1 + g_2 \int K_1(z') dz' > 0 \), if the density is large, only a small band values of \( \hat{k} \) would be modulationally unstable.

The modulational band, where instability occurs, is better understood in Figure 3.5, where \( u_0 = \) controls the parabolic curve, shown as a dash-dotted line, and the nonlinear
constants control the bell shape, shown in red. As $u_0$ increase, the width of the parabola increases. As $g_1$ increase, the curve of the Fourier Transform of the dipolar kernel moves vertically up. The value of $g_2$ determines the concavity of the curve for $g_2\mathcal{K}(\hat{k})$. For $g_2$ negative, a large value of $g_1$ would be required to have $H(\hat{k})$ function to be positive. Once $g_1 + g_2\mathcal{K}(0)$, a small band appears in the center of the wavenumber space for which $H > 0$. For large values of $\omega_\perp$, we required large value for the nonlinearity constants as well as large values of $u_0$ to have a homogeneous background to be unstable.
Figure 3.3. The modulation gain of dipolar BEC $g_1 = 1$ and $g_2 = -5$. Background density changes between 0.05 and 4, and wave number lies in the interval $(-1, 1)$. The modulational gain is quite large even when the density is quite small.

Figure 3.4. The modulation gain of dipolar BEC $g_1 = -1$ and $g_2 = \frac{5}{\pi}$. Background density between 0.05 and 4, and wave number from $-2$ to 2. The gain only occurs for relatively large value of background density $u_0$. 
Figure 3.5. Factor of the modulation gain that determines the band of M.I. is the function \( H \). The dash-dotted (blue) line represents the parabola whose width depends on the background \( u_0 \). The dash (red) line represents the \( g_1 + g_2 \mathcal{K}(\hat{k}) \) factor where \( \omega_\perp = 200 \). Here \( u \approx 5.8, g_2 = 1, \) and \( g_1 \approx -23 \).
CHAPTER 4
NUMERICAL METHODS

In this chapter we describe the numerical algorithms used to find steady states of the dipolar GP equation. We also discuss the algorithms used to simulate and detect dark soliton formation to test our predictions. The same algorithms are used to test the growth rate of perturbations of the homogeneous background, obtained from the MI analysis.

In all the numerical algorithms, we discretize space in a regular grid with a grid size of \( \Delta z \). The discretization of the one-dimensional interval \( \Pi = [-L, L] \) is done with \( N + 1 \) points so that \( z_i = -L + i\Delta z \) where \( i = 1, 2, \ldots, N + 1 \). Because the FFT algorithm is used for the calculation of the Fourier space, we should have \( N + 1 \) to be a large integer power of 2 for fast and efficient computation. The length \( L \) takes values from 100 to 250. As mentioned in Chap. 1, the width of a dark soliton, placed on a background of density \( |\rho_0|^2 \), can be measured by the healing length \( \xi = 1/\sqrt{2|\rho_0|^2 g_1} \). Thus, one must choose \( \Delta z \leq \xi \) to allow for several points to describe the dark soliton core. For example, if \( L = 210 \), \( g_2 = 0 \) and \( g_1 = 4 \), a dark soliton has a healing length \( \xi \approx 0.3535 \), and then we require more than \( N + 1 > 2^{11} = 2048 \) points to create a grid that properly resolve dark solitons with \( \Delta z \approx 0.2051 \).

Time is similarly discretized, where the initial time is zero so that \( t_n = n\Delta t \). Using this discretization, we have:

\[
u_i^n \equiv \psi_i^n,
\]

where \( \psi_i^n \in \mathbb{C} \). It is clear that the external potential \( V_{1D} \) and the dipolar kernel \( K_1 \) are also discretized. The boundary conditions play a special role both in the numerical approximations of the steady state as well as in the numerical time integrations; thus, Section 4.3 in this chapter will be dedicated to this issue.
4.1 Finding the Steady States of the Dipolar GP Equation

To find the steady states of the dipolar GP equation, we start by using the time-independent form of the dipolar GP equation:

$$\mu u = -\frac{1}{2} \nabla^2 u + V_{1D} u + g_1 |u|^2 u + g_2 [K_1 * |u|^2] u,$$  \hspace{1cm} (4.1)

where $[K_1 * |u|^2] = \int K_1 (r - r') |u(r')|^2 dr'$, and $V_{1D}(z) = \frac{1}{2} \omega_z^2 z^2$. The model uses a complex partial integro-differential equation which adds a certain difficulty to finding a steady state.

Thus, to find steady states, we look for roots of the function

$$F(u) = -\frac{1}{2} \nabla^2 u + V_{1D} u - \mu u + g_1 |u|^2 u + g_2 [K_1 * |u|^2] u,$$  \hspace{1cm} (4.2)

which is a tedious task even in 1D. It is clear that $u \equiv 0$ is a trivial root, then we look for nonzero solutions to the discretization of Eq. (4.2). The Laplacian operator is discretized using the finite difference method. The operator is called the discrete Laplacian operator, as denoted using $\Delta_i$, and the order of this approximation is denote here by the sub-index $i$. The second order approximation using the two neighboring grid points is:

$$\Delta_2 v_i = \frac{v_{i-1} - 2v_i + v_{i+1}}{\Delta z^2},$$

which satisfies $\nabla^2 u(z_i) = \Delta_2 v_i + O(\Delta z^2)$. If we seek a higher order approximation, we can use for example the fourth order approximation. In that case, $\nabla^2 u(z_i) = \Delta_4 v_i + O(\Delta z^4)$, where

$$\Delta_4 v_i = -v_{i-1} + 16v_{i-1} - 30v_i + 16v_{i+1} - v_{i+2}.\Delta z^2.$$

The convolution (integral term) can be written as a (left) Riemann sum:

$$[K_1 * |v|^2](z_i) \approx \sum_{l=1}^{N} K_1(z_i - z_l)|v_l|^2 dz$$

Thus, to find a the steady state we need to solve the discretization of Eq. (4.2), that is a system of equations in the form of:

$$F_i = -\frac{1}{2} \frac{v_{i-1} - 2v_i + v_{i+1}}{\Delta z^2} + (V_{1D}(z_i) - \mu + g_1 |v_i|^2 + g_2 \sum_{l=1}^{N} K_1(z_i - z_l)|v_l|^2 dz) v_i = 0,$$  \hspace{1cm} (4.3)

for $i = 2, \ldots N$. The boundary conditions determine the behavior of $v_1$ and $v_{N+1}$. The boundary condition as well as the initial iteration is discussed in Section 4.3.
4.1.1 The Newton-Rhapson Method

The Newton-Rhapson method, deduced from the multivariable Taylor expansion, is an iterative method that focuses on solving the roots of a function $F$, $F(\vec{x}) = 0$, by calculating from an initial guess $\vec{x}_0$. The next iteration is expressed as $\vec{x}_{k+1} = \vec{x}_k + \vec{s}_k$ where the Newton step is given by $\vec{s}_k = -J_F(\vec{x}_k)^{-1}F(\vec{x}_k)$, which is the solution to the linear system $J_F(\vec{x}_k)\vec{s} = -F(\vec{x}_k)$. The term $J_F(\vec{x}_k)$ is the Jacobian matrix of the function evaluated at the previous iterative. Without knowing the exact root, the algorithm stops when the relative norm of the residual is below a determined tolerance, $\|F(\vec{x}_k)\| \leq \tau_1\|F(\vec{x}_0)\|$, or a sufficiently small Newton step: $\|\vec{s}_k\| \leq \tau_2\|\vec{x}_0\|$ where the constants $\tau_i$ correspond to the desired tolerances.

Due to the complex nature of $u$, the system to be solved must consider the real and imaginary part of $v$. Let $J_F$ be the discretized version of the Jacobian matrix of Eq. (4.1). Basically, we solve for a system of $2(N+1)$ equations following Eq. (4.3). The first $N+1$ equations of the system will represent the real part of $F_i$ and the next $N+1$ represent the imaginary parts of the same expression. Therefore, the Jacobian can be expressed by

$$J_F = \begin{bmatrix} \frac{\partial R(F_i)}{\partial R(v_j)} & \frac{\partial \Im(F_i)}{\partial R(v_j)} \\ \frac{\partial R(F_i)}{\partial \Im(v_j)} & \frac{\partial \Im(F_i)}{\partial \Im(v_j)} \end{bmatrix}. \quad (4.4)$$

The Jacobian matrix for $F$ may also be written in the form: $J_F = J_1 + J_2 + J_3 + J_4$, where each matrix $J_i$ represents the Jacobian of the discrete Laplacian, the potential term, local term and the dipolar term respectively. The size of each Jacobian matrix, $2(N+1) \times 2(N+1)$, becomes larger as the number of points in the grid increase. Thereby, the Jacobian for the discretize Laplacian of the second order is a block matrix with two triangular matrices in the diagonal:

$$J_1 = \begin{pmatrix} J_c & 0 \\ 0 & J_c \end{pmatrix}$$

$$J_c = -\frac{1}{2 \Delta z^2} \begin{pmatrix} b_1 & -2 & 1 \\ 1 & -2 & 1 \\ & \ddots & \ddots & \ddots \\ & & 1 & -2 & 1 \\ & & & 1 & -2 & 1 \\ b_{N+1} & & & & & \end{pmatrix}, \quad (4.5)$$

where the boundary conditions determine the entries at the corners of each $J_c$ matrix.
If the identity matrix of size $N + 1$ is denoted by $I_{N+1}$, then $J_2$ will be a similar block matrix with the scalar matrix that holds $(V_1D(z_i) - \mu)I_{N+1}$ in the diagonal blocks. As for the cubic term of the local interaction, we have that $|v_i|^2 = \Re(v_i)^2 + \Im(v_i)^2$. Then

\[
|v_i|^2 v_i = (\Re(v_i)^2 + \Im(v_i)^2)\Re(v_i) + i(\Re(v_i)^2 + \Im(v_i)^2)\Im(v_i)
\]

\[
= \Re(v_i)^3 + \Im(v_i)^2\Re(v_i) + i(\Re(v_i)^2\Im(v_i) + \Im(v_i)^3)
\]

(4.6)

The matrix corresponding to the local term is then:

\[
J_3 = g_1 \begin{bmatrix} M_1 & M_2 \\ M_2 & M_3 \end{bmatrix}, \tag{4.7}
\]

where

\[
M_1 = (3\Re(v_i)^2 + \Im(v_i)^2) I_{N+1},
\]

\[
M_3 = (\Re(v_i)^2 + 3\Im(v_i)^2) I_{N+1}, \tag{4.8}
\]

\[
M_2 = (2\Re(v_i)\Im(v_i)) I_{N+1}.
\]

A direct approach on the dipolar term in Eq. (4.3) will make the Jacobian a full matrix, given that each $v_i$ is affected by every other point $v_j$ through the following convolution:

\[
\sum_{l=1}^{N} K_1(z_i - z_l)|v_l|^2 \quad v_i = K_1(z_i - z_1)(\Re(v_1)^2 + \Im(v_1)^2)(\Re(v_i) + i\Im(v_i)) + K_1(z_i - z_2)(\Re(v_2)^2 + \Im(v_2)^2)(\Re(v_i) + i\Im(v_i)) + \ldots + K_1(z_i - z_N)(\Re(v_N)^2 + \Im(v_N)^2)(\Re(v_i) + i\Im(v_i)) + K_1(z_i - z_{N+1})(\Re(v_{N+1})^2 + \Im(v_{N+1})^2)(\Re(v_i) + i\Im(v_i)).
\]

(4.9)

Let us denote $K_i(l) = K_1(z_i - z_l)$. We can write the entries of the Jacobian matrix $J_4$ in vector form. For example the first $N + 1$ rows of the matrix have the form

\[
g_2 \cdot \Delta z \cdot ([\overrightarrow{R}_1 0] + [0 \overrightarrow{R}_2]).
\]

The first vector $\overrightarrow{R}_1$ of size $(N + 1)$ is given by the derivative of the real part of Eq. (4.9) according to the real parts at each point.

\[
\overrightarrow{R}_1 = [2K_i(1)\Re(v_1)\Re(v_i) \quad 2K_i(2)\Re(v_2)\Re(v_i) \quad \ldots \quad (\sum_{l=1}^{N-1} K_i(l)|v_j|^2) + K_i(i)(3\Re(v_i)^2 + \Im(v_i)^2) + \sum_{i+1}^{N+1} K_i(j)|v_j|^2] \tag{4.10}
\]

\[
\ldots \quad 2K_i(N)\Re(v_N)\Re(v_i) \quad 2K_i(N+1)\Re(v_{N+1})\Re(v_i)],
\]

where only the $i$-th entry of the vector is different. Similarly $\overrightarrow{R}_2$ is the derivative of the real part of Eq. (4.9) according to the imaginary part of each point:

\[
\overrightarrow{R}_2 = [2K_i(1)\Im(v_1)\Re(v_i) \quad 2K_i(2)\Im(v_2)\Re(v_i) \quad \ldots \quad K_i(i)(2\Re(v_i)\Im(v_i)) \quad K_i(i)(2\Re(v_i)\Im(v_i)) \quad \ldots \quad 2K_i(N)\Im(v_N)\Re(v_i) \quad 2K_i(N+1)\Im(v_{N+1})\Re(v_i)].
\]

(4.11)
We can write the second set of $N+1$ row vectors as: $-g_2 \cdot \Delta z \cdot ([\vec{R}_3^\ast 0] + [0 \vec{R}_4^\ast])$. The vector $\vec{R}_3^\ast$ is given by the derivative of the imaginary part of Eq. (4.9) according to the real parts at each point:

$$\vec{R}_3 = [2K_i(1)\mathcal{R}(v_i)\mathcal{I}(v_i) \ 2K_i(2)\mathcal{R}(v_i)\mathcal{I}(v_i) \ \cdots \ K_i(i)\mathcal{R}(v_i)\mathcal{I}(v_i)]$$

(4.12)

and similarly $\vec{R}_4^\ast$ is the derivative of the imaginary part of Eq. (4.9) according to the imaginary part of each point:

$$\vec{R}_4 = [2K_i(1)\mathcal{I}(v_i)\mathcal{I}(v_i) \ 2K_i(2)\mathcal{I}(v_i)\mathcal{I}(v_i) \ \cdots \ K_i(i)\mathcal{I}(v_i)\mathcal{I}(v_i)]$$

(4.13)

Notice that $\vec{R}_2 = 2\mathcal{R}(v_i)K_i\mathcal{I}(v_i)$, and $\vec{R}_3 = 2\mathcal{I}(v_i)K_i\mathcal{R}(v_i)$. We can quickly make the other two row vectors by constructing $\vec{R}_1 = 2\mathcal{R}(v_i)K_i\mathcal{R}(v_i)$, and $\vec{R}_4 = 2\mathcal{I}(v_i)K_i\mathcal{I}(v_i)$. We will need to modify the $i$-th coordinate, by using

$$\langle \vec{R}_{1,4} \rangle_i = \sum_{j=1}^{N+1} K_i(j)|v_j|^2 + K_i(i)(-|v_i|^2 + a\mathcal{R}(v_i)^2 + b\mathcal{I}(v_i)^2))$$

Finally, the convolution term $[\int K_1(z - z')|v(z')|^2dz']v$ can lead to a highly dense Jacobian matrix. All the entries of the Jacobian matrix depend on the iteration $v_i$. Thus, for large matrix sizes the loading process can consume some time. Even when the condition number is not large, solving the linear system with a full matrix is computationally-intensive. Another approach is not to fully discretize the convolution term and hold constant the calculation $\int K_1(z - z')|v(z')|^2dz'$ on every iteration, hence, the matrix $J_4$ would be a scalar matrix.

Neither approach guarantees the convergence of Newton’s method towards the steady state. In the regime of modulational instability for example, the Newton algorithm can converge to the trivial solution $v \equiv 0$ or completely fail to converge. The matrix size of the matrix is large, even for one-dimensional case, the Newton-Rhapson method may encounter storage problems. Therefore, a more reliable algorithm is needed in those cases. The Newton-Krylov is a good candidate since it can be written as a free-matrix procedure, which is described in the next section.
4.1.2 The Newton-Krylov Method

A Newton-Krylov solver finds the Newton step \( \vec{s} \) but focuses more on an inexact Newton condition:

\[
\| J_F(\vec{x}_n)\vec{s} + F(\vec{x}_n) \| \leq \eta \| F(\vec{x}_n) \|
\]

where the scalar parameter, \( \eta \), determines the local convergence of the inexact Newton algorithm. This parameter can also be updated on each iteration and bounded away from 1, which guarantees at least linear convergence [25]. After the vector \( \vec{s} \) is found, good optimization algorithms can use a linear search to find the next iteration:

\[
\vec{x}_{n+1} = \vec{x}_n + \alpha \vec{s}
\]

until \( \| F(\vec{x}) \| \leq \tau_r \| F(\vec{x}_0) \| + \tau_a \), where \( \tau_r \) and \( \tau_a \) are the relative and absolute tolerances.

The generalized minimal residual method (GMRes), or other Krylov space methods, can be used to solve for the Newton direction, \( \vec{s} \), from the linear system \( J_F(\vec{x}_n)\vec{s} = -F(\vec{x}_n) \). Krylov methods focus on solving the linear system \( A\vec{x} = \vec{b} \), using matrix-vector multiplication of the form \( A\vec{w} \), instead of matrix-matrix operations. In numerical linear algebra, Krylov methods are among the most successful algorithms because results from previous matrix-vector multiplications are used to search for the solution. The GMRes(m) has the advantage of being a low-storage iterative method that restarts a GMRes after \( m \) iterations using the result of a previous GMRes run as the initial guess.

Another notable property of the Newton-Krylov algorithm is that it can be written as a matrix-free algorithm. The operation \( J_F(\vec{x}_n)\vec{w} \), which is done repeatedly, is approximated with a forward difference directional derivative.

\[
J_F(\vec{x})\vec{w} \approx D_h F(x : w) = \begin{cases} 
0 & \vec{w} = \vec{0} \\
\| \vec{w} \| \frac{F(\vec{x} + h \| \vec{w} \| \vec{w}) - F(\vec{x})}{h \| \vec{w} \|} & \vec{x} \neq \vec{0} \\
\| \vec{w} \| \frac{F(h \| \vec{w} \| \vec{w}) - F(\vec{x})}{h} & \vec{x} = \vec{0}
\end{cases}
\]

To solve complex nonlinear equations, we use the MATLAB package \texttt{nso1i} , which can be found in Ref. [33]. The package implements the GMRes(m) algorithm to solve a linear system \( A\vec{x} = \vec{b} \) where \( A \) is an \( N \times N \) matrix. The GMRes algorithm itself is an iterative numerical method that approximates the solution starting from an initial iteration \( \vec{x}_0 \) that could be the zero vector or the result of a previous GMRes process, minimizing the residual \( \vec{r} = \vec{b} - A\vec{x}_n \). Each new iteration is generated from previous iterations. The method terminates when either the maximum number of iterations is reached or \( \| \vec{b} - A\vec{x}_n \|_2 \leq \eta \| \vec{b} \|_2 \), which allows for control of the forcing term as an inexact Newton method.
In mathematical terms the $k$-th iterate of the GMRes satisfies: $\vec{x}_k \in \vec{x}_0 + \mathbb{K}_k$, where $\mathbb{K}_k = \text{span}\{\vec{r}_0, A\vec{r}_0, \ldots A^{k-1}\vec{r}_0\}$ is the Krylov subspace. We look to minimize the norm of the residual over the Krylov subspace:

$$\left\| A\vec{x}_k - \vec{b} \right\| = \min_{\vec{x} \in \vec{x}_0 + \mathbb{K}_k} \left\| \vec{b} - A\vec{x} \right\| .$$

Many theorems can be proven about the GMRes; most of them rely on the following theorem. Define the set of $k$-th degree residual polynomials as the set

$$\mathcal{P}_k = \{ p | p(x) = \sum_{j=0}^{k} a_j x^j, p(0) = a_0 = 1 \} .$$

**Theorem 4.1.** Let $A$ be a nonsingular matrix, and let $\vec{x}_k$ be the $k$-th GMRes iteration. Then,

$$\left\| \vec{r}_k \right\| = \min_{p \in \mathcal{P}_k} \left\| p(A)\vec{r}_0 \right\| \leq \left\| \hat{p}(A)\vec{r}_0 \right\| \quad \forall \hat{p} \in \mathcal{P}_k .$$

As a corollary, if matrix $A$ of size $N \times N$ is nonsingular, the GMRes can find the solution within $N$ iterations. Also, if $A$ has $m$ distinct eigenvalues, then the algorithm terminates at most in $m$ iterations. The GMRes can be referred to as a direct method since it can find the solution, but this idea is only possible in infinite precision. A numerical solution can be found after $N$ iterations, but it might not be accurate. The algorithm can also stop at a given number of iterations and can calculate an approximate solution very easily. This is not possible with a direct method like Gauss elimination.

The GMRes was introduced on Ref. [54] while the authors were investigating for methods to solve linear systems with non-symmetric matrices. A direct approach would required to solve on each iteration the linear system like $B_k\vec{x} = \vec{y}$, with the Krylov matrix: $B_k = [\vec{r}_0, A\vec{r}_0, \ldots A^{k-1}\vec{r}_0]$. The storage and the QR factorization of such matrix becomes expensive and it has to be performed on every new iterate. However, one may use the Gram-Schmidt orthogonalization to efficiently solve the linear system $A\vec{x} = \vec{b}$ without restarting the QR factorization on each iteration.

By means of the Arnoldi iteration, the sequence of orthonormal vectors that span the Krylov subspace are generated. The process is quite stable and easier when using the Gram-Schmidt process to find the orthogonal projection onto $\mathbb{K}_k$ as a matrix $V_k$, such that every $\vec{z} \in \mathbb{K}_k$ can be written as a linear combination of the columns of $V_k$. Therefore, $\vec{x} \in \vec{x}_0 + \mathbb{K}_k$ has a form $\vec{x} = \vec{x}_0 + V_k\vec{y}$. The method starts with the first column as $\vec{v}_1 = \frac{1}{\|\vec{r}_0\|}\vec{r}_0$.

Given the previous $k$ orthonormal vectors, i.e. the columns of $V_k$, finding the next orthonormal vector, satisfies $AV_k = V_{k+1}\hat{H}_k$ where $\hat{H}_k$ is a $k + 1 \times k$ Hessenberg matrix,
which is a matrix with zeros below the first sub-diagonal. This has the exceptional advantage of using the previously calculated columns. The Arnoldi iteration has then:

\[
\vec{v}_{i+1} = A\vec{v}_i - \sum_{j=1}^{i} ((A\vec{v}_i)^T \vec{v}_j) \vec{v}_j / \| A\vec{v}_i - \sum_{j=1}^{i} ((A\vec{v}_i)^T \vec{v}_j) \vec{v}_j \|.
\]

If the \(i\)-th column of \(V_k\) is the unitary vector in the direction of the \(i\)-th Arnoldi vector. Rather, a stable Gram-Schmidt process is used to slowly construct \(\hat{H}_k\). The next vector \(\vec{w}_{i+1} = A\vec{v}_i\) is used temporarily, and as suggested by the stabilized Gram-Schimdt process, a loop around the previous vectors is performed, \(j = 1, 2, \ldots, i\). The projection over the previous vectors is eliminated:

\[
\vec{w}_{i+1} = \vec{w}_{i+1} - (\vec{w}_{i+1} \cdot \vec{v}_j) \vec{v}_j.
\]

The coefficients of \(\hat{H}_k\) are constructed at the same time as dot products between the new vector and the previous columns of \(V_k\) as it progresses through the loop:

\[
\langle \hat{H}_k \rangle_{ji} = (\vec{w}_{i+1})^T \vec{v}_j.
\]

Finally the resulting vector is normalized:

\[
\langle \hat{H}_k \rangle_{i+1} = \| \vec{w}_{i+1} \| \vec{w}_{i+1} / \| \vec{w}_{i+1} \|.
\]

An intuitive breakdown of such algorithm is the possible breakdown caused by the iteration that can cause a division by zero, but this is not a disadvantage in this case because of the following lemma:

**Lemma 4.1.** Let \(A\) be nonsingular matrix; let \(\vec{v}_j\) be the vectors generated by Arnoldi’s algorithm; lset \(i\) be the smallest integer such that:

\[
A\vec{v}_i - \sum_{j=1}^{i} ((A\vec{v}_i)^T \vec{v}_j) \vec{v}_j = \vec{0},
\]

then \(\vec{x} = A^{-1} \vec{b} \in \vec{x}_0 + \mathbb{K} \mathbb{L}_i\).

The general idea of the proof of this lemma has a useful notation: Denote \(\beta = \| \vec{r}_0 \|\), then \(\vec{r}_0 = \beta V_k \vec{e}_1\) for any \(k\) iteration. Given the hypothesis of the lemma, \(AV_i = V_i H_i\), where \(V_i \in \mathbb{R}^{N \times i}\) is the matrix of orthonormal vectors that generate the Krylov Subspace. Here \(H_i\) is a square Hessenberg matrix. Notice now that by calculating the norm of the \(i\)-th residual can be done without explicitly determining \(\vec{x}_i\):

\[
\| \vec{r}_i \|_2 = \| \vec{r}_0 - A(\vec{x}_i - \vec{x}_0) \|_2 = \| V_i \beta \vec{e}_1 - AV_i \vec{y} \|_2
\]

\[
= \| V_i (\beta \vec{e}_1 - H_i \vec{y}) \|_2 = \| \beta \vec{e}_1 - H_i \vec{y} \|_{\mathbb{R}^{i+1}}.
\]

Thus, \(\vec{y} = \beta H_i^{-1} \vec{e}_1 \in \mathbb{R}^i\), generates an exact solution at the \(i\)-th iteration for \(\vec{x}_i = \vec{x}_0 + V_i \vec{y}\).

The naive idea is to stop the GMRes at each iteration and measure the residual. Here, we discuss the power of the the GMRes to avoid calculating the residual directly. The \(k\)-th iteration can be found by first solving \(\hat{H}_k \vec{y} = \beta \vec{e}_1\), in the \(\mathbb{R}^k\) space. Then \(\vec{x}_k = \vec{x}_0 + V_k \vec{y}\). The square matrix \(H_k\) has a Hessenberg form, that is \(H_k \in \mathbb{R}^{k \times k}\), which has zero entries below the
first sub-diagonal. Although the Arnoldi algorithm does not produce a full upper triangular matrix, a Hessenberg is often the next best thing when solving linear systems.

The Givens rotations will transform the entries in the first sub-diagonal of $\tilde{H}_k$ into zero. The QR factorization of $\tilde{H}_k$ constructs $Q^T = G_k G_{k-1} \ldots G_1$ as an orthogonal matrix constructed by a series of Givens matrices such that $Q^T \tilde{H}_k = \tilde{R}_k$ is an upper triangular matrix. The first Given matrix satisfies $\tilde{R}_1 = G_1 \tilde{H}_k$ and has a nonzero entry in the first column only in the diagonal, by construction. The Givens matrix $G_j(c, s) \in \mathbb{R}^{k+1 \times k+1}$ will not change the first $j$-th columns of $\tilde{R}_{j-1}$ when calculating $\tilde{R}_j = G_j \tilde{R}_{j-1}$. The matrix has the following form:

$$G_j(c_j, s_j) = \begin{bmatrix}
1 & 0 & \cdots & 0 \\
0 & \ddots & \ddots & \vdots \\
& \ddots & 1 & 0 \\
& & 0 & c_j - s_j \\
& & s_j & c_j & 0 \\
& & & \ddots & \ddots \\
0 & \cdots & 0 & 1
\end{bmatrix}. \tag{4.15}$$

At the end of the Givens rotations process a triangular matrix $R_k$ of size $k + 1 \times k$ can be found, where the last row of $\tilde{R}_k$ is zero, so it is rather useful to work with the square part, $R_k$. The idea is to minimize the function:

$$J(\vec{y}) = \| \beta \vec{e}_1 - \tilde{H}_k \vec{y} \| = \| Q^T (\beta \vec{c}_1 - \tilde{H}_k \vec{y}) \| = \| \vec{g} - R_k \vec{y} \|,$$

where $\vec{g} = \beta Q^T \vec{c}_1 \in \mathbb{R}^{k+1}$ and whose last element is zero, hence, it is better to work with its first $k$ values, $\hat{\vec{g}}$. Thereby, the new iterative needs to solve $R_k \vec{y} = \hat{\vec{g}}$, or simply $\tilde{R}_k \vec{y} = \hat{\vec{g}}$. The $k$ iteration is then $\vec{x}_k = \vec{x}_0 + V_k \vec{y}$.

As the algorithm progresses on each iteration $i$, an updated version of $H_i$ can store the triangular form $R_i$ after performing the Givens rotations. The Givens rotations can be performed by accessing the values of $c_i$ and $s_i$ for each rotation. Thus, those values are only the information required and not the full Givens matrix. The rotation is applied to the previous information of $H$, whose previous columns are a triangular sub-matrix. The rotation is also done to the $\beta \vec{c}_1$ to obtain $\vec{g}$. The interesting fact, is that now the current norm of the residual at the last iteration can be found without the calculation of $\vec{x}_k$. The residual norm is $\| \vec{r}_k \| = \| \vec{g}_k - R_k \vec{y}_k \|$ but, by construction of $\vec{y}_k$, this is equal to the absolute value of the last component of $\vec{g}_k$, $|g_k|$. A tolerance for the norm of the residual can be established using the
norm of $\vec{b}$. Hence, the algorithm stops when $|g_k| \leq \epsilon \|\vec{b}\|$ where $\epsilon \ll 1$.

Likewise, one of the important factors is the fact that the Givens rotations can be performed by storing only the information from the coefficients $c_j$ and $s_j$. The algorithm is also very easy to program computationally where only a small amount of matrices are stored. In essence only two new matrices are required to be saved, $V_k$ and the triangular matrix $R_k$. It was shown that a solution can be found within $m < N$ iterations, where $m$ is the number of distinct eigenvalues. But this again may be too large because the size of the two matrices is determined by the number of iterations $m$.

Given that orthogonalization is an essential part of the Arnoldi method, it is a good idea to verify whether the Gram-Schimdt process may have formed non-orthogonal vectors due to imprecision. This of course will break the algorithm because the identity $\|\vec{r}\| = \|\beta\vec{e}_1 - H_k\vec{y}\|$ is no longer valid because the reduction of the Hessenberg matrix is inaccurate. A second orthogonalization is possible, but not recommended in every iteration. A Brown/Hindmarsh condition can be used as test, so that orthogonalization is done twice if after the first orthogonalization $\|\vec{v}_{k+1}\| \ll 1$, or numerically $\|\vec{v}_k\| + \delta \|\vec{v}_{k+1}\| \approx \|\vec{v}_k\|$. Thus, the size or dimension of the matrices $V_k$ and $R_k$ can be established at the start of the algorithm. In theory, the norm of the residual decreases monotonically, but it could just as well decrease very slowly. Although the decrease may occur in the last $N$ iterations, the GMRes algorithm behaves very well when the eigenvalues are grouped together in a few clusters near 1. GMRes(m) is a code that restarts the GMRes method after $m$ iterations, and uses the result from the previous GMRes as the initial iteration.

In the unusual case that the GMRes algorithm does not converge, the nSoli has other Krylov methods such as the BiCGSTAB and the TFQRM to solve for the linear system. The N-Soli has control over the forcing term $\eta$ and guarantees at least linear convergence of the inexact Newton method. Finally, the full Newton step $\vec{s}$ should not always be taken. The nSoli uses a three-point parabolic model for the line search to find the root in the direction of the Newton step. The next iteration $\vec{x}_{n+1} = \vec{x}_n + \lambda \vec{d}$ is chosen such that a decrease in $\|F\|$ is guaranteed, where $\lambda$ is the step length to be determined. The line search should not be ignored as it prevents the algorithm from finding another root by overshooting and it counteracts possible oscillations.

The stopping criteria for the N-Soli are controlled by the norm of the initial iteration. The N-soli ends when $\|F(\vec{x})\| \leq \tau_T = \tau_r \|F(\vec{x}_0)\| + \tau_a$ or a maximum number of iterations.
is reached. Now, the construction of a large matrix $J$ can be avoided, and only the function of Eq. (4.3) is needed. But now, a better approximation can be used instead; for example the fourth-order discrete Laplacian $\Delta_4$ and a more precise numerical integration for the convolution term. The left Riemann sum is only an estimation of the integration. We implemented a composite Simpson’s rule, which works great since the discretization of space is made with an even number of points. The final result $w^0$, if within numerical tolerance, should be the steady state, the root of Eq. (4.1).

### 4.2 Time Integration of the Dipolar GP Equation

We first wrote Eq. (2.26) as a discrete ordinary differential equation (ODE):

$$f(t, v) = \frac{\partial v}{\partial t} = -i \left( -\frac{1}{2} \Delta v + V_{1D}(r, t)v + g_1|v|^2v + g_2 \left[ K_1 * |v|^2 \right] v \right). \quad (4.16)$$

The numerical time integration of Eq. (4.16) consists of an approximation of the flow of the differential model. The flow $\varphi$ of an autonomous differential equation is given by:

$$\begin{cases} \dot{x}(t) = F(x(t)) \\ x(t_0) = x_0 \end{cases}$$

that is $\varphi_t(x_0) = x(t)$. For a time dependent flow in the dipolar GP Eq. (4.16), it can still be considered an autonomous flow by the simple trick of writing: $G(t, v) \equiv (1, f(t, v))$ and $y(t) \equiv (t + t_0, v(t))$ Then, the flow is now

$$\begin{cases} \dot{y}(s) = G(y(s)) \\ y(0) = (t_0, v_0) \end{cases}$$

The first approach to integrate Section 4.2 is to use an explicit algorithm, such as the Runge-Kutta. When dealing with the convolution term, the integration becomes very difficult and requires storing of a large amount of information if done in the space domain $\Pi$. The Fourier transform allows for a way to calculate the dipolar term, in the Fourier space:

$$\mathcal{F}[(K_1 * u^2)(x)](\hat{k}) = \mathcal{K} \cdot \mathcal{F}[u(x)](\hat{k}), \quad (4.17)$$

where $\mathcal{K}$ is the Fourier transform of the dipolar kernel $K_1$. Therefore, we transform the function back and forth between the real and Fourier space, and multiplied by the fixed function (in Fourier space) $\mathcal{K}$. Numerical FFT algorithms that find the Fourier transform are most efficient when the number of points in the space discretization is a power of 2.
Explicit numerical methods approximate the solution of the next time step \( \Upsilon[h](y_0) \approx y(t_0 + h) \), where \( h = \Delta t \) by only using the information on the previous step. Other numerical methods that solve for an implicit function exist, that is \( y(t_0 + h) = G(y_0, y(t_0 + h)) \) but such algorithms are not recommended with a dipolar GP equation, because the convolution term is already hard to calculate.

As a matter of fact, given that the density is transformed to the Fourier space, a pseudo-spectral time-split algorithm can be used to approximate the flow [5, 60, 63]. A simulation of a non-autonomous ODE, such as Eq. (4.16), can be seen as
\[
if(t, v) = i\frac{\partial v_1}{\partial t} + i\frac{\partial v_2}{\partial t},
\]
that means a combination of two ODE’s that have an exact solution:
\[
\begin{align*}
\frac{i}{\partial t} v_1 &= -\frac{1}{2} \Delta v_1 \\
\frac{i}{\partial t} v_2 &= \tilde{V}(\vec{x}, t) v_2 + g_1 |v_2|^2 v_2 + g_2 (K_1 * |v_2|^2) v_2.
\end{align*}
\]
In the following subsections, we quickly describe the Runge-Kutta method, a very well known explicit method for numerical integration for ODEs, and the Strang-Marchuk algorithm, a pseudo-spectral time-split algorithm that allows for the construction of numerical methods of higher order.

### 4.2.1 Standard Explicit Runge-Kutta

A standard explicit fourth-order Runge-Kutta (RK) is used to simulate the time integration of the ODE given in Eq. (4.16). The discretization in time is done with a time step of \( \Delta t \), where by diffusion conditions the size of the time step should be in the same order as the square of the space grid size: \( \Delta t < \Delta z^2 \). The next time step is calculated by:
\[
v^{n+1} \approx \Upsilon_{RK}[h](v^n) = v^n + \frac{1}{6} \Delta t (k_1 + 2k_2 + 2k_3 + k_4)
\]
where the \( k_i \) terms are:
\[
\begin{align*}
k_1 &= f(t_n, v_n), \\
k_2 &= f(t_n + \frac{1}{2} \Delta t, v_n + \frac{1}{2} \Delta tk_1), \\
k_3 &= f(t_n + \frac{1}{2} \Delta t, v_n + \frac{1}{2} \Delta tk_2), \\
k_4 &= f(t_n + \Delta t, v_n + \Delta tk_3).
\end{align*}
\]

The RK method allows for the potential to be time dependent, but a drastic change in the impurity velocity could lead to unexpected behavior and radiation because it could add some momentum to the condensate. The moving potential should increase its initial velocity of zero to \( \nu \) adiabatically, namely the potential should slowly increase its velocity and avoid
adding a considerable amount of energy into the system. Thus, the center of the impurity at time \( t_1 \) is chosen to be: 
\[
p(t_1) = p(t_0 + \Delta t) = p(t_0) + \Delta t \cdot \nu \frac{1 + \tanh(\sigma \cdot t_1)}{2} \]
where \( \sigma \) accounts for the width of the time required for the velocity to change from zero to \( \nu \) as mentioned in Section 2.4.

The non-autonomous nature of the GP equation with a moving potential requires the time step to be small. Simulations show that the Runge-Kutta is stable for \( \Delta t \approx \kappa \Delta z^2 \) with \( \kappa = 0.05 \).

### 4.2.2 The Strang-Marchuk Algorithm

Using the properties of the Fourier transform, we can write the first ODE in Eq. (4.18) as:

\[
i \frac{\partial \hat{v}_1}{\partial t} = -\frac{1}{2} (2\pi i \hat{k})^2 \hat{v}_1,
\]
where the discrete Fourier transform, of the discrete iteration \( v^n \), will be denoted by \( \hat{v}^n = \mathcal{F}[v^n](\hat{k}) \). Working with the Fourier transform imposes an immediate requirement: the boundary conditions need to be periodic. However, this is not a great issue in the presence of an external trap, where \( \omega_z \neq 0 \), given that the density of the condensate decays towards zero in such cases.

If \( v^n \) is the \( n \)-th time iteration, we can find \( \Upsilon_{\text{Strang}}[h](v^n) = v^{n+1} \), the approximation of the wave-function at the next time step \( t_{n+1} = (n + 1)\Delta n \) by performing the following three steps from the Strang-Marchuk method. In the dipolar GP model, these are:

1. First, numerically solve the first equation of Eq. (4.18) with a step size of \( \Delta t \) using as the initial condition \( v_1(0) = v^n \)

\[
v^n_{\frac{1}{2}}(z) = \mathcal{F}^{-1}\left[\exp(-i \frac{\Delta t}{2} |2\pi \hat{k}|^2 )\mathcal{F}[v^n](\hat{k})\right](z),
\]
where \( v^n_{\frac{1}{2}} \) denotes an intermediate step.

2. Numerically solve the second equation of Eq. (4.18) with a step size of \( \Delta t \), but in this case use the previous result as the initial condition: \( v_2(0) = v^n_{\frac{1}{2}} \)

\[
v^n_{\frac{3}{2}}(\vec{x}) = \exp(-i \Delta t(V_{1D}(z, t) + g_1 |v^n_{\frac{1}{2}}|^2 + g_2 [\mathcal{K} \ast \rho](\vec{x}) \right) v^n_{\frac{1}{2}}.
\]

The convolution term can be calculated by using the Fourier transform of the density of the initial condition \( \rho = |v^n_{\frac{1}{2}}|^2 \):

\[
[\mathcal{K} \ast \rho](\vec{x}) = \mathcal{F}^{-1}(\mathcal{K} \cdot \mathcal{F}[|v^n_{\frac{1}{2}}|^2](\hat{k})).
\]
3. To obtain the numerical approximation of the wave function at time $t_{n+1} = (n + 1)\Delta t$, the first ODE is solved one more time with a step size of $\frac{\Delta t}{2}$ but using the previous intermediate result as the initial condition, $v_{1}(0) = v_{\frac{n}{2}}^{n}$:

$$
v_{n+1}^{n+1} = \mathcal{F}^{-1} \left[ \exp\left(-\frac{i}{2} \frac{\Delta t}{2} |2\pi \hat{k}|^{2}\right) \mathcal{F} \left[ v_{\frac{n}{2}}^{n} \right] \left( \hat{k} \right) \right](z).
$$

### 4.2.3 Higher Order Split-Time Methods

The previous Strang method can be proven to be an unconditionally stable second-order algorithm [45]. The Strang method can be easily modified to have higher-order accuracy. The flow $\varphi_t$ of a differential equation: $\dot{y} = f(y)$, such as in Section 4.2, is defined as the mapping that advances the solution by time $t$. A general property of a flow is that it satisfies $\varphi_{-t} = \varphi$. In most numerical methods this does not occur. The adjoint of a numerical method is defined as the inverse of the original map in reverse time: $\Upsilon_{h}^{*} \equiv \Upsilon_{-h}^{-1}$. A symmetric method satisfies $\Upsilon_{h}^{*} = \Upsilon_{h}$ and its order is always even. That is

$$
\Upsilon[h](y_0) = \varphi_h(y_0) + O(h^{2s+1}) + O(h^{2s+2}).
$$

Using this notation, we can construct a composition of $s$ time-split methods (each of order $r$) with different time steps. The method defined by $\Xi_h = \Upsilon[\gamma sh] \circ \ldots \circ \Upsilon[\gamma_1 h]$ is of order $r + 1$ if:

$$
\begin{align*}
\sum_{i=1}^{s} \gamma_i &= \gamma_1 + \ldots + \gamma_s = 1 \\
\sum_{i=1}^{s} \gamma_i^{r+1} &= \gamma_1^{r+1} + \ldots + \gamma_s^{r+1} = 0.
\end{align*}
$$

The equations on (4.20) have no particular solution for $r$ odd or when $s \leq 2$. But when the composition is constructed out of symmetric methods, the composite method would also be symmetric and in fact of an even order larger than $r + 1$. For the Strang-split method, the order is 2, $r = 2$. We can find a symmetric method of fourth-order via the composition of 3 Strang-split methods: $s = 3$. For simplicity $\gamma_1 = \gamma_3 = \gamma$ and $\gamma_2 = 1 - 2\gamma$ allows the previous conditions to be satisfied if $\gamma = \frac{1}{3} \left( 2 + 2^{\frac{1}{2}} + 2^{-\frac{1}{3}} \right)$.

The previous procedure can be repeated to obtained higher-order methods and it can be used to find a reference solution since we lack the exact solution for the dipolar GP model. Methods to construct a higher-order method are available. We used the composition provided on Ref. [44], consisting of 15 Strang-split method, where the coefficients for the time step.
length are:

\[
\begin{align*}
\gamma_1 &= 0.74167036435061295344822780, & \gamma_{15} &= \gamma_1, \\
\gamma_2 &= -0.40910082580003159399730010, & \gamma_{14} &= \gamma_2, \\
\gamma_3 &= 0.19075471029623837995387626, & \gamma_{13} &= \gamma_3, \\
\gamma_4 &= -0.5738624711160826665638773, & \gamma_{12} &= \gamma_4, \\
\gamma_5 &= 0.2990641813036559238446354, & \gamma_{11} &= \gamma_5, \\
\gamma_6 &= 0.33462491824529818378495798, & \gamma_{10} &= \gamma_6, \\
\gamma_7 &= 0.31529309239676659663205666, & \gamma_9 &= \gamma_7, \\
\gamma_8 &= -0.79688793935291635401978884.
\end{align*}
\]  

\[4.21\]

Among the advantages of such methods is the fact that the scalars can easily be stored, as well as the factor \(\exp\left(\frac{-i}{2} \Delta t \gamma_i \right)\) that is needed twice for each Strang step.

### 4.3 Other Important Calculations

As mentioned before, we used from the discretization of Eq. (4.2), yields

\[
F_i = -\frac{1}{2} \Delta_4 v_i + (V_{1D}(z_i) - \mu + g_1 |v_i|^2 + g_2 \sum_{l=1}^{N} K_1(z_i - z_l)|v_l|^2 dz) v_i \equiv 0,
\]

for \(i = 2, \ldots, N\). We need to discuss is the behavior at the boundary, \(v_0\) and \(v_{N+1}\), for both numerical problems: solving the steady state and the time integration. The boundary conditions depend directly on the existence of the external potential. Another issue that arises is the calculation of the convolution close to the boundary. In this section we discuss the necessary size for the domain, the value \(L\). We also need to determine the initial iteration that will be use to find the steady state of the dipolar GP.

#### 4.3.1 Boundary Conditions

When the harmonic trap is present, the trap strength along the longitudinal direction is nonzero (\(\omega_z \neq 0\)) and the condensate is localized in the center of the trap. There is a slow variation of the density away from the center. For nondipolar BEC, where \(g_2 = 0\), an approximation of the ground state system solves Eq. (4.2) but neglecting the spatial derivative. In such situations: \(\rho(z) \approx \frac{\mu - V_{1D}(z)}{g_1}\). The distance \(R_{TF} = \sqrt{2\mu/\omega_z}\) is known as the Thomas-Fermi radius, where the (nondipolar) density of the condensate is zero, \(\rho(R_{TF}) = 0\). For the dipolar condensates, the size of the cloud could either compress or expand due to the nonlocal forces of the dipolar. We denoted \(R_c\) as the radius of dipolar condensate, and it was not predetermined. We may find the steady state for a very large domain \(1 \ll L\), and obtain
the value of $R_e$ for each different configuration of the parameter values for further simulations.

In the case $\omega_z \neq 0$, the density of the condensate decreases to zero outside of the region of interest, $|z| \leq R_e$, we used a Dirichlet condition for the boundaries: $u(z) = 0$ if $z \in \partial \Pi$. Thus, in the discretization, we use $v_1 = 0$ and $v_{N+1} = 0$ as the boundary conditions for the Newton methods used in finding the steady state. This boundary condition can also be used for the numerical simulations of the time integration.

In case that the setting requires a constant background density $\rho$ at the boundary, such as the cases of $\omega_z = 0$, then the boundary condition is $|u(z)|^2 = \rho_0$ for $z \in \partial \Pi$. In the case that we seek a stationary soliton, we set the boundary as seen in the condition of the dark soliton in the NLS Eq. (1.17). Therefore, $v_1 = \sqrt{\rho} = -v_{N+1}$ is the boundary condition for the Newton methods. For homogeneous constant backgrounds we merely need $v_i = \sqrt{\rho}$ for $i = 1, \ldots N + 1$, but in those cases we do not need to perform the Newton algorithm.

For time integration, the boundary condition is not as trivial when the harmonic trap is absent. We cannot set the values of $v_1$ and $v_{N+1}$ to a fixed value due to the rotational nature of the wave-function $u$. In such cases, we use the modulus-square Dirichlet (MSD) boundary condition suggested in Ref. [10]. The relation

$$\frac{\partial u}{\partial t}(z_b) \approx i\Im \left( \frac{\partial u}{\partial t}(z_{b+1}) \frac{1}{u_{b+1}} \right) u(z_b).$$

allows us to approximate the time derivative at a point in the boundary, $z_b$ with information at a neighbor interior point $z_{b+1}$. This method is ideal for RK algorithms, given that these algorithms calculate $u_t$ explicitly. The MSD boundary condition is recommended only for non-zero background; the algorithm fails if the density at the boundary is very close to zero.

The use of the pseudo spectral scheme imposes a periodic boundary condition. In the setting where a constant density is required this algorithm is not recommended. For example the real part of a dark soliton in the one-dimensional NLS does not satisfy periodic boundary conditions. Indeed, the density is equal to 1 at both extremes, but while one boundary can be at the value 1, the other is at the value $-1$. In these cases, the RK with the MSD method is much preferred.

For our numerical studies, the size of cloud should have a large radius such that the impurity does not leave the condensate before nucleation occurs, thus, the size of the domain requires $R_e < L$. Another important factor that determines the size of the domain is the
precision of the calculation of the convolution. The convolution is defined as the integration of the product between two function as one of those is reversed and shifted.

\[ [K_1 * |u|^2](z) = \int K_1(z' - z)|u(z')|^2 \, dz' \]  (4.22)

In the case that \( |u(z)|^2 \) does not decay, the calculation of the convolution might be inexact because part of the information is lost on the other side of the boundary. Hence, when \( |u|^2 \) is a homogeneous background density, we assume that the convolution within a certain region of the boundary is the same as the convolution at the inner neighboring point. The region is determined by the reach of the dipolar kernel \( K_1 \). As mentioned before, let \( z_b \) be the point at the boundary, and \( z_{b+1} \) the nearest inner neighbor. Thus, if \( K_1(z_{\text{max}}) \ll 1 \), then

\[ [K_1 * |u|^2](z_k) \xrightarrow{\text{set}} [K_1 * |u|^2](z_{b+1} \pm 2z_{\text{max}}) \]  (4.23)

where \( z_k \) is relatively close to the boundary: \( |z_k - z_b| \leq z_{\text{max}} \). Therefore, to keep this calculation from disrupting our simulations, the size of the domain needs to be considerably large.

### 4.3.2 Initial Estimate for Newton Methods

The initial guess cannot be arbitrary because both root-finding algorithms, Newton-Rhapson and Newton-Krylov are not global methods. The initial guess has to be a good estimate. The initial guess is constructed based on the setting of the external harmonic trap along the longitudinal direction, control by the frequency \( \omega_z \). Another factor is whether we want to start our simulation with a soliton already located in the center of the condensate or not.

For example, to find a stationary dark soliton over a homogeneous background, where \( \omega_z = 0 \), we use, as pointed out by the analytical solution of the NLS Eq. (1.16), an initial guess should be:

\[ v(z) = \rho_0 \tanh(\rho_0(z - z_0)) \exp(ikz), \]  

where \( |\rho_0|^2 \) is the density at which the dark soliton is seeded.

For the setting where there is the presence of an external trap, \( \omega_z \neq 0 \), we used an approximation of the ground state. The Thomas-Fermi (TF) approximation requires neglecting the Laplacian term in Eq. (2.26) and, thereby,

\[ |u(z)|^2 \approx (g_1 + g_2 \int K_1(z) \, dz)^{-1}(\mu - V_{1D}(z)) \]  

where \( \mu - V_{1D}(z) > 0 \). It is also quite trivial to place a soliton in the center of the cloud, by multiplying the profile of a dark soliton with background 1 and the Thomas-Fermi cloud.
Once the steady state is found, denoted by \( w^0 \), we perturb the numerical solution by adding some small perturbation, because we are never physically on the correct steady state. Therefore, we add a random vector with complex entries \( z^0 \).

\[
v^0 = w^0 + z^0.
\]

This will be used as an initial condition for the time integrations.

### 4.3.3 Calculating Phase-Shift

As time integration occurs, we can calculate each component of the energy, that is the energy of the system due only to kinetic energy, potential energy, and, local and nonlocal interaction energy. Because our interest is to determine the nucleation of dark solitons, we look for phase-shifts close to the value of \( \pi \). Given that one or more dark solitons may be nucleated, we measure the changes in the arguments on an interval of sizes similar to the width of a soliton. Given the fact that the healing length is denoted by \( \xi \), we can find dark soliton by numerically looking for where the phase-shift \( S(z) \approx \phi(z + \frac{\xi}{2}) - \phi(z - \frac{\xi}{2}) \), is close to \( \pi \).

What we have listed is a set of numerical algorithms well-suited for our purposes. The time-split algorithms are certainly more accessible for fast computations in case that the external trapping is present, \( \omega z \neq 0 \), since in those cases, the interpolation of the dipolar term is not required at the boundary. The Newton-Krylov package is a great algorithm that can solve the root of a nonlinear equation, and it will be used not just to find the steady states but can also be used to solve differential equations we will see in the following chapter.
CHAPTER 5
ANALYSIS AND PREDICTIONS FOR THE CRITICAL VELOCITY

The speed of sound describes the natural velocity of excitations, or sound waves. Thus, an impurity moving at velocities above the speed of sound, \( v_s \), may cause instability in the medium [46]. Experimentally, this is the approach taken to nucleate dark solitons and vortices in one- and two-dimensional BECs. But numerically we can find that there are velocities just below the speed of sound, at which dark solitons are nucleated.

Now that the model for the one-dimensional dipolar GP equation has been described, and that the parameter region \((g_1, g_2)\) where homogeneous backgrounds are stable has been identified, we can seek for the critical velocity at which dark solitons will nucleate as a spatially localized potential travels through the condensate.

Next we describe the analytical approach to find the speed of sound and the differential equations that will allow us to find the critical velocity, \( v_c \). We follow the analysis described in Ref. [31]. We consider a homogeneous condensate with constant density which is modulationally stable according to the previous chapter and an impurity that moves at a velocity \( \nu \) across the condensate.

5.1 THEORETICAL PREDICTION

For the mathematical approach, the one-dimensional form of the dipolar GP Eq. (1.14) is given by:

\[
i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \frac{\partial^2 \psi}{\partial z^2} + V_{1D}(z, t) \psi + g_1 |\psi|^2 \psi + g_2 \left( \int K_1(z - z') |\psi(z')|^2 \, dz' \right) \psi.
\] (5.1)

If there is no external harmonic potential, what remains is a impurity that moves at a speed \( \nu \). Therefore, the external potential takes the form \( V_{1D}(z, t) = V_{\text{imp}}(z - \nu t) \), where the impurity is chosen as the narrow Gaussian:

\[
V_{\text{imp}}(z - \nu t) = \beta \sqrt{\frac{2}{\pi \sigma}} \exp \left( -\frac{(z - \nu t)^2}{2 \sigma^2} \right).
\] (5.2)

The boundary condition for a constant background, \( |\psi|^2 = \rho \), is enforced. A stable constant density solution can be found for the GP equation, Eq. (2.10) with \( g_2 = 0 \), only if the
nonlinear term $g_1$ is positive. It was previously shown that for $g_1 < 0$, constant densities are unstable. Within the context of BECs, a repulsive nonlinearity allows for the existence of stable backgrounds. In the dipolar GP equation, stability conditions are required from both the nonlinear constant $g_1$ and the dipolar term $g_2$, to have stable solutions with constant background. As a minimum requirement, $\mu(g_1 + g_2[\int K_1(r') \, dr']) > 0$, as discussed in the previous chapter.

The following analysis relies on a co-moving reference frame. Therefore, we use a Galilean transformation for the solution, $\psi(\vec{x}, t) = \psi(\vec{x}, t) \exp(-i\mu t)$, so that the frequency parameter, $\mu$, appears explicitly in the differential equation.

$$i \frac{\partial \psi}{\partial t} + \frac{1}{2} \nabla^2 \psi - V_{\text{imp}}(x - \nu t) \psi + \mu \psi - g_1|\psi|^2 \psi - g_2[\int K_1(z - z')|\psi(z')|^2 \, dz'] \psi = 0. \quad (5.3)$$

Then, the change of reference is performed: $u(\xi, \tau) = \psi(\xi + \nu \tau, \tau)$, where $\xi = z - \nu t$ and $\tau = t$:

$$u_z = u_\xi \frac{\partial \xi}{\partial z} + u_\tau \frac{\partial \tau}{\partial z} = u_\xi,$$

$$u_t = u_\xi \frac{\partial \xi}{\partial t} + u_\tau \frac{\partial \tau}{\partial t} = -\nu u_\xi + u_\tau.$$

The dipolar GP in the co-moving reference frame is then given by:

$$-i\nu u_\xi + i u_\tau + \frac{1}{2} u_{\xi\xi} - V_{\text{imp}}(\xi) u + \mu u - g_1|u|^2 u - g_2 \left[ \int K_1(\xi - \xi')|u(\xi')|^2 \, d\xi' \right] u = 0. \quad (5.4)$$

The dipolar term is not affected by the co-moving frame because the integration is conducted over the infinite real line. With the variable substitution $\xi' = r' - \nu \tau$:

$$\left[ \int K_1(z - z')|\psi(z', t)|^2 \, dz' \right] \psi(z, t) = \left[ \int K_1(\xi + \nu \tau - r')|\psi(r', \tau)|^2 \, dr' \right] \psi(\xi + \nu \tau, \tau) = \left[ \int K_1(\xi - \xi')|u(\xi', \tau)|^2 \, d\xi' \right] u(\xi, \tau).$$

Equation (5.4) now describes the flow of a dipolar GP equation, whose external potential is the impurity fixed at $\xi = 0$. In the non-dipolar BEC ($g_2 = 0$), a flow of constant density at velocity $\nu$ evolves in three different ways depending on $\nu$:

- For velocities above the speed of sound, grey solitons will be emitted from the peak of the disturbance.
- At very low speeds, a stable steady flow (state) can be found.
• There is a transitional state to the creation of grey solitons at larger velocities that can coexist with the steady flow close to critical velocity. The two steady states disappear in a saddle-node bifurcation so that no steady flow can be found above the critical velocity.

Let us take a steady state solution of the form \( u(\xi) = R(\xi) \exp(i\phi(\xi)) \). The time-independent solution, \( u_\tau = 0 \), yields two equations, one for the real part and another for the imaginary part: these are respectively:

\[
-\nu R \phi' = \frac{1}{2} (R'' - R(\phi')^2) - V_{\text{imp}} R + \mu R - g_1 R^3 - g_2 \left[ K_1 * R^2 \right] R, \tag{5.5a}
\]

and

\[
\nu R' = \frac{1}{2} (2R' \phi' + R\phi''). \tag{5.5b}
\]

The imaginary part of the time-independent solution can be integrated to obtained a differential equation on the derivative of the phase function, \( \phi \), using the boundary condition \( |u|^2 = \rho \):

\[
2\nu R' = 2R' \phi' + R\phi'' \quad \Rightarrow \quad (2\nu - 2\phi') R' = R\phi''
\]

\[
\frac{R'}{R} = \frac{(\phi')'}{2\nu - 2\phi'} \quad \Rightarrow \quad -\frac{1}{2} \ln(2\nu - 2\phi') = \ln(R) + C
\]

\[
\ln(R^{-2}) = \ln(2\nu - 2\phi') + 2C \quad \Rightarrow \quad 2\nu - 2\phi' = KR^{-2}
\]

\[
\phi' = 0 \text{ and } R^2 = \rho \text{ at } |\xi| = \infty \quad \Rightarrow \quad 2\rho \nu = K
\]

\[
\Rightarrow \phi' = \nu (1 - \frac{\rho}{R^2}). \tag{5.6}
\]

For now, the exact solution to \( \phi \) is not necessary, but if the differential Eq. (5.6) is replaced into the real part of the time-independent expression (5.5a), we obtain the main equation of this chapter:

\[
\frac{1}{2} R'' = \nu^2 \left( \frac{\rho^2}{R^3} - R \right) + V_{\text{imp}} R - \mu R + g_1 R^3 + g_2 \left[ \int K_1(\xi - \xi') R^2(\xi') d\xi' \right] R. \tag{5.7}
\]

Far from the center \( \xi = 0 \) where the impurity is located, there is a possibility for a stable constant background. Notice that if \( R^2 = \rho \), as required by the boundary condition, then Eq. (5.7) is satisfied if and only if \( \mu = \rho (g_1 + g_2 \int K_1(z') dz') \). This is the relationship between the chemical potential, the background density and the nonlinear constants. As mentioned before in Chap. 2, the dipolar kernel, \( K_1 \), can be approximated by a \( \delta \) function when \( \omega_r \) is large. Under such a consideration, the convolution term is a linear operator, leaving only the integration of the dipolar kernel as a scalar factor. For this reason we denoted \( G = g_1 + g_2 \int K_1(z') dz' \) as the unique nonlinearity constant. This parameter will play a critical role in the approach of the following section, as well as determining the speed of
sound.

We can obtain the speed of sound, $v_s$, using linear perturbation. Let us linearize Eq. (5.7) around a perturbed constant steady state: $R(\xi) = \sqrt{\rho} + \epsilon r(\xi)$ where $\rho$ is a real positive value and consider $V_{imp}$ to be zero:

$$
R = \sqrt{\rho} + \epsilon r + O(\epsilon^2), \quad R^3 = \rho^{3/2} + 3\rho \epsilon r + O(\epsilon^2), \quad R' = \epsilon r' + O(\epsilon^2).
$$

(5.8)

The dipolar term is also expanded as it was done in Chap. 3:

$$
\left[\int K_1(\xi - \xi')|\sqrt{\rho} + \epsilon r(\xi')|^2 d\xi'\right] (\sqrt{\rho} + \epsilon r(\xi)) = [K_1 * \rho](\sqrt{\rho}) + \epsilon \rho \left[ K_1 * (\overline{r} + r) + \int K_1(z') dz' (r) \right] + O(\epsilon^2)
$$

$$
\approx [K_1 * \rho](\sqrt{\rho}) + \epsilon \rho (3r) \left[ \int K_1(z') dz' \right] + O(\epsilon^2).
$$

If the linear perturbation is expanded in Eq. (5.7), the following differential equation is obtained:

$$
\frac{1}{2} \epsilon r'' = \frac{\nu^2}{2} (4\epsilon r) - \mu \epsilon r + 3 g_1 \rho \epsilon r + 3 g_2 \rho \epsilon \left[ \int K_1(\xi') d\xi' \right] r + O(\epsilon^2).
$$

Because $\mu = \rho (g_1 + g_2 \int K_1(z') dz') = \rho G$, we obtain the following ODE for the steady state perturbation:

$$
\nu'' = 4(\mu - \nu^2) r.
$$

What we have obtained is a second-order linear ODE for the steady state perturbation when $|\xi| \gg 1$. There are 4 oscillating modes, 2 for large positive values of $\xi$ and 2 for large negative values of $\xi$. For solutions to the differential equation of $r$ without any oscillations, i.e. stable, to be possible yields $\mu - \nu^2 > 0$. Thus, the speed of sound is $v_s = \sqrt{\mu}$. Following the same analysis of Ref. [31], we find that the only possibility for non-oscillating solutions and to keep the divergent mode to zero, is to consider a localized solution. Without the exact solutions to Eq. (5.7), we are only able to continue our analysis considering short-range potentials or numerical approximations. The former approach is considered in the following section.

### 5.2 Short-Range Impurity Potential

The analytical approach taken here is to consider $V_{imp}$, the potential of the moving impurity, to be of short range compared to the healing length of the GP. Let us then consider
$V_{\text{imp}}(\xi) = \beta \delta(\xi)$, a delta potential of strength $\beta$. This approach will allow for an estimate of the critical velocity.

In this case, the differential equation for the amplitude of the steady state solution reads:

$$\frac{1}{2} R'' = \frac{\nu^2}{2} \left( \frac{\rho^2}{R^3} - R \right) + \beta \delta(\xi) R - \mu R + GR^3. \quad (5.9)$$

For $\xi \neq 0$ we can find two solutions to this differential equation, with a free parameter $\xi_0$, which have a hyperbolic profile given by:

$$R^2(x) = \frac{\nu^2}{G} + \left( \rho - \frac{\nu^2}{G} \right) \tanh^2 \left( \sqrt{G} \sqrt{\rho - \frac{\nu^2}{G}} (\xi \pm \xi_0) \right) \quad \text{for } x \geq 0. \quad (5.10)$$

The profile of such stationary solutions is depicted in Figure 5.1, where the nonlinearity constant is $G = 1$, the background density is set to 1, the impurity strength is $\beta = 2$, and the velocity of the co-moving reference frame is $\nu = 0.2$, which we will show is below the critical velocity.

**Figure 5.1. Solutions of Eq. (5.9), where $G = 1$ and $(\nu, \beta) = (0.2, 0.5)$. These are the steady states of the co-moving reference frame with a $\delta$-impurity. The stable solution is shown with the solid (blue) line and the unstable is shown with the dotted (red) line.**

The differential Eq. (5.9), introduces a jump condition close to the center $\xi = 0$. Taking into consideration the stationary solution of Eq. (5.4), the limit of the integral around the center of the impurity, $\xi \approx 0$, results in a jump discontinuity of the spatial derivative:

$$\lim_{\epsilon \to 0} \int_{0+\epsilon}^{0+0} \frac{1}{2} u_{\xi\xi} \, d\xi = \lim_{\epsilon \to 0} \int_{0+\epsilon}^{0+0} \beta \delta(\xi) u \, d\xi.$$

$$\lim_{\epsilon \to 0} \int_{0+\epsilon}^{0+0} \frac{1}{2} u_{\xi\xi} \, d\xi = \lim_{\epsilon \to 0} \int_{0+\epsilon}^{0+0} \beta \delta(\xi) u \, d\xi. \quad (5.11)$$
The jump condition, Eq. (5.11), relates the parameter of the solutions $\xi_0$ with the strength of the impurity $\beta$, and its velocity $\nu$. This relationship will allow us to find the critical velocity $v_c$ for the short-range potential. The right hand of the jump condition is $2\beta u(0)$. Since $u = R \exp(i\phi)$, the spacial derivative satisfies $u' = R' \exp(i\phi) + i\phi'R \exp(i\phi)$. Dividing the previous expression by $u(0)$, yields a calculation for $2\beta$ as:

$$
\frac{u'}{u}\Big|^{0+}_{0-} = \frac{R'}{R} + i\phi' \Big|^{0+}_{0-} = \frac{2RR'}{R^2} (\xi = 0^+) - \frac{2RR'}{R^2} (\xi = 0^-). \tag{5.12}
$$

The imaginary part of Eq. (5.12) is easily eliminated because $\phi'$ is even. Therefore, we obtain the relationship:

$$
\beta = \sqrt{G} (\rho - \frac{\nu^2}{G})^{\frac{3}{2}} \tanh(\sqrt{G} \sqrt{\rho - \frac{\nu^2}{G} \xi_0}). \tag{5.13}
$$

As we can see in Figure 5.2, one may notice that in Eq. (5.13) as the parameter of the solution $\xi_0$ increases, the strength of the impurity, $\beta$, increases to a maximum and then tends back to zero. For a fixed velocity $\nu < v_c$, and if $\beta$ is below the maximum, there are two possible values for $\xi_0$. Each describes a steady state of the co-moving reference frame of the homogeneous BEC with an impurity. As the velocity is increased, the two steady states disappear in a saddle-node bifurcation. Thus, at this velocity, there is only one value for $\xi_0$, denoted as $\xi_c$, which determines the maximum value of $\beta$ in Eq. (5.13). This maximum is shown as the solid line on top of the curve in Figure 5.2.

The maximum is found by differentiating with respect to $\xi_0$, and setting the result equal to zero allowing us to determine the critical value $\xi_c$. This procedure yields

$$
\beta = \text{sech}^2(\sqrt{G} \sqrt{\rho - \frac{\nu^2}{G} \xi_c}), \tag{5.14}
$$

which when replaced back into the original Eq. (5.13), establishes $\beta$ as a function of the critical velocity $v_c$:

$$
\beta = 2\sqrt{\frac{\nu^2}{\mu}} \left(1 - \frac{\nu^2}{\mu} \right) \sqrt{\frac{1 + \frac{\nu^2}{\mu} - \left(1 + 2\frac{\nu^2}{\mu} \right)}{\left(4\frac{\nu^2}{\mu} - 1 \right) + \sqrt{1 + \frac{8\nu^2}{\mu}}}. \tag{5.14}
$$

The other parameters, such as background density and the effective nonlinearity constant are contained in $\mu = \rho G$. Thus, increasing the background has the same effect as increasing the effective nonlinearity constant. The relationship in Eq. (5.14) is satisfied but it
will not allow us to easily determine the critical velocity as a function of $\beta$. We can only determine through series expansion, a direct relationship of $\beta$ and $v_c$. We can show that

$$1 - \frac{v_c^2}{\mu} = \frac{2}{\sqrt{\mu}}(\sqrt{\mu} - v_c) - \frac{1}{\mu}(\sqrt{\mu} - v_c)^2,$$

which means that the first factor $1 - \frac{v_c^2}{\mu}$ vanishes as $v_c$ approaches the speed of sound, $v_s = \sqrt{\mu}$. A series expansion of $v_c$ around the speed of sound, $v_s = \sqrt{\mu}$, for both the numerator and denominator of the quotient in Eq. (5.14) allows us to determine that right hand side vanishes like $(\sqrt{\mu} - v_c)^{\frac{3}{2}}$. Finally, we have that

$$\beta \approx C(\sqrt{\mu} - v_c)^{\frac{3}{2}},$$

(5.15)

where $C$ is determined by the constant of the zero order terms: $C = \frac{4}{9}\frac{\sqrt{6}}{\mu^\frac{1}{2}}$. Thus, close to the critical velocity, the short-range potential approach yields

$$v_c \approx \sqrt{\mu} - 2^{\frac{1}{4}}\frac{3\mu^{\frac{1}{4}}}{4}(\beta)^{\frac{3}{4}} \quad \beta \ll 1.$$

(5.16)

As the strength of the impurity increases, the critical velocity tends to zero, decreasing proportional to $1/\beta$. Using a series expansion around zero instead, one obtains:

$$v_c \approx \frac{\mu}{2\beta} \quad \beta \gg 1.$$  

(5.17)
Such approximations are a direct result when the dipolar kernel is assumed to have a \( \delta \)-function approximation. In Figure 5.3, we depict an example of the relationship given by Eq. (5.14), as well as the approximation for small and large impurity strengths.

**Figure 5.3.** The solid (blue) line corresponds to the relationship between the critical velocity \( v_c \) vs. \( \beta \), the strength of the impurity. In this case, the effective nonlinearity is \( G = 2 \), and the density of the background is \( \sqrt{\rho} = 2 \), thus, \( \mu = 4 \). The dash-dotted (green) line corresponds to the approximation of the critical velocity in the case of small values of \( \beta \). The dash (red) line corresponds to the case when \( \beta \) is large.
In this chapter we present the numerical calculations and time integrations for the one-dimensional dipolar GP equation. We validate the results of the modulational gain, that is, the growth rate of perturbations of the homogeneous background. We determined the region of modulationally instability for a constant background of 1 based on the modulational gain function obtained in Chap. 3. This is compared with the linear approximation, where the effective nonlinearity is given by $G = g_1 + g_1 \int K_1(z') \, dz'$. Finally, we simulate dark soliton nucleation over a set of configurations for the parameter values of $g_1$ and $g_2$. We compare the results of the critical velocity predicted analytically with the ones obtained from our numerical integrations.

For our discretization of space and time, we consider the conditions described in Chap. 4. We investigate the behavior of the dark soliton nucleation considering different values of the nonlinear constant. We consider as well two values of $\omega_\perp$, the trapping frequency in the transverse direction. The first value is $\omega_\perp = 2$, thus the dipolar kernel is proportional to the kernel presented in Ref. [17]. In general, for quasi-one dimensional BEC, the trapping frequency in the transverse direction is around 100 times stronger than the frequency in the longitudinal direction [28]. Thus, we also consider $\omega_\perp = 100$, and found that in such cases the simulations agree with the analytical results obtained before.

### 6.1 Integration for Modulational Instabilities

In this section, we focus on the time integration of a modulationally unstable homogeneous steady states. We verify that the calculation of the modulational gain, i.e. our perturbation and stability analysis, is valid in the linear regime. Recall that in the case of nondipolar BEC, the nonlinear constant $g_1$ fully determines the modulationally stability of the one-dimensional GP equation. Thus, we compare the modualtional gain vs. the effective nonlinearity constant $G$ that arises when the convolution behaves like a linear operator.

First, consider the case where the effective nonlinearity is negative: $g_1 + g_2 \int K_1(z') \, dz' < 0$. We begin by considering the absence of the external potential, that is
ω_z = 0. For the numerical simulations, we rely in the explicit RK methods with a finite central difference to integrate Eq. (4.16), and since the background has a constant density at the boundary, we make use of the MSD boundary condition method described in Section 4.3.1. We studied analytically the perturbation of a homogeneous steady state with background of density 1:

\[ \psi_0 = 1 + (a \exp(2\pi i \hat{k}z) + b \exp(-2\pi i \hat{k}z)), \]  

(6.1)

where \( a \) and \( b \) represent the amplitude of the perturbation. Numerically, when we add noise to the constant density, we are adding a perturbation with random values of \( \hat{k} \). In order to measure the growth rate, we calculate the relative norm from the initial state:

\[ \Delta U(t) = \frac{\|u(t) - \psi_0\|}{\|\psi_0\|}, \]

and the slope in the semi-log scale would reveal the largest growth rate. Figure 6.1 depicts a particular example where \( g_1 = 1 \) and \( g_2 = -\frac{5}{\pi} \). Given the values of the nonlinear constants, we can calculate the modulational gain using Eq. (3.13). For a constant density of 1, the largest modulational gain is 1.4038. In the numerical simulation, the density saturates very quickly, thus the calculation of the norm will be unreliable after that. The exponential growth of the perturbation can still be seen with in the first few seconds of the simulation.

Figure 6.1. Example of the growth rate computation using a small perturbation of the constant density 1. Here, \( g_1 = 1 \) and \( g_2 = -\frac{5}{\pi} \). The maximal modulational gain is approximately 1.403, same as the slope of the (green) line shown here.
6.2 Region of Parameters for Modulational Stable Backgrounds

In Chap. 5, we found the behavior of the modulational gain function is given by
\[ \Lambda(\hat{k}) = 2\pi |u_0 \hat{k}|^2 \Re(\sqrt{-H}), \]
where \( H \) is the function
\[
H(\hat{k}, g_1, g_2, u_0) = g_1 + g_2 \mathcal{K}(\hat{k}) + \left( \frac{\pi \hat{k}}{u_0} \right)^2,
\] (6.2)
and \( \mathcal{K} \) is the Fourier transform of the nonlocal dipolar kernel, \( K_1 \). For modulationally stability, we need the expression of \( H \) to be positive.

From \( H \), we can predict a region of the parameter space \((g_1, g_2)\) where the homogeneous backgrounds are modulationally stable. We can say that the effective nonlinearity \( G = g_1 + g_2 \int K_1(z') \, dz' \) measures the modulational gain at \( \hat{k} = 0 \). We establish here an approximate criteria for the modulational instability: The line \( x = -y \left( \int K_1(z') \, dz' \right) \), which might provide some insight to the behavior of stability in the parameter region \((g_1, g_2)\).

Setting the background to the fixed value of 1 and the fact that \( \mathcal{K} \) decays towards zero for large values of \( \hat{k} \), we can determine the stability for every point \((g_1, g_2)\) of the plane by simply numerically calculating the maximum of the modulational gain. We start with \( \omega_\perp = 100 \), Figure 6.2, and notice that the bifurcation line is parallel to the criteria described above.

![Figure 6.2](image)

**Figure 6.2.** The dotted (blue) line represents the line \( y = -x \int K_1(z') \, dz' \). The top right area (shown in green) represents the \((g_1, g_2)\) parameter space where homogeneous states are modulationally stable.
When $\omega_z$ is relatively small, we calculate the bifurcation curve in the plane $(g_1, g_2)$ for infinitesimal perturbations of the constant density. It resembles a line with negative slope passing close to the origin. Therefore, we can obtain a region with competing nonlinearities to use for further simulations. Notice in Figure 6.3 that the bifurcation curve is no longer parallel to the line $x = -y(\int K_1(z') dz')$. There are regions between the previous line and the bifurcation curve where results do not agree. We calculated the modulational gain for a parameter set within that region. We studied the two cases, where the region of bifurcation does not match to the region determined by the expected line. For the cases $(g_1 = -5, g_2 = 3)$ and $(g_1 = 5, g_2 = -3)$, we plotted the factors of $H$ to confirm the instability in Fig. 6.4 respectively. Thus, the bifurcation criterion proves to be close to the real bifurcation line for large values of $\omega_\perp$, where the dipolar kernel becomes more local.

Figure 6.3. The dotted (blue) line represents the expected bifurcation line given by $x = -y\int K_1(z') dz'$. The bifurcation curve is calculated from the modulational gain, where the stability starts to change.
Figure 6.4. The dashed (blue) curve describes the parabola given by $\pi^2 \hat{k}^2$. The dashed (red) corresponds to $g_1 + g_2 \Re(\hat{k})$. The two graphs show the curve for $H$ for the case of $\omega_\perp = 2$. The graph on the left corresponds to $g_1 = -5$ and $g_2 = 3$, and the graph on the right corresponds to $g_1 = 5$ and $g_2 = -3$; both located in the region of conflict.

6.3 Stationary Solutions

Before the numerical integration is performed, we study the steady states of the dark solitons. The nonlocality generates dark soliton very similar to the nondipolar cases, but around the center of the soliton small humps are formed when there is repulsive nonlocal interaction. In general, the width of the dark soliton increases when the local repulsive interaction is increased. We studied the phase-shift that occurs at the center of all dark solitons, because this determines the criteria to find them numerically later on. The phase-shift change that occurs at the center is still close to $\pi$ for all. We can compare several dark solitons found through the Newton nonlinear solver in Figure 6.5.

Figure 6.5. Dipolar dark solitons: $(g_1, 5/\pi g_2)$: $(5, -1)$, $(-1, 1)$ and $(0, 1)$ in blue, red and green respectively. The non-dipolar dark soliton is shown magenta: $(1, 0)$. 
We can also find the steady states where the impurity is present (but stationary) using the Newton-Krylov. We also performed time integrations for such situations to corroborate the calculation of mass, energy, as well as determining the frequency of rotation of the real and imaginary part. The height of the cloud cannot be fixed at 1 because the Newton method uses the parameter $\mu = G$ where $G$ is the effective nonlinear constant. See Fig. 6.6 for a snapshot of a particular example of a dipolar BEC with $g_1 = -1, g_2 = 0.1$ where the external harmonic trap is present and the impurity is fixed at $x = 0$. The behavior for the same configuration over a time lapse of 70 seconds is shown in Fig. 6.7. The real and imaginary parts of the wave function for all steady states found rotate at the rate $\frac{2\pi\omega}{\mu}$.

![Graph showing wave function behavior](image)

**Figure 6.6.** This is a snapshot of the dipolar condensate where the impurity does not move. The green and red line correspond to the real and imaginary part of the wavefunction respectively. The blue line corresponds to the density of the condensate. The amplitude of the impurity is $A = 0.1$. This is configuration 8, where $g_1 = -1, g_2 = 0.1$ for $\omega_\perp = 100$. 
Figure 6.7. The graph on the left represent the rotation of the real (green) and imaginary (red) part for a stationary solution with a dark soliton inside a harmonic trap. The graph of the right is the difference of mass (cyan) and total energy (blue) from their respective mean. The amplitude of the fixed impurity is $A = 0.1$ for a time interval of 70 seconds. This is configuration 8, where $g_1 = -1, g_2 = 0.1$ for $\omega_\perp = 100$, thus $\frac{2\pi}{\mu} = 10.5463$.

6.4 INTEGRATION OF THE FULL ONE-DIMENSIONAL DIPOLAR GP EQUATION

We selected 10 different configuration settings for the nucleation of dark solitons. In Fig. 6.8, we can view that the configurations are within the region of modulational stability. On Table 6.1, we show the table of important value for each of the configurations. The speed of sound is given by $\sqrt{\mu}$, which is directly related to the background density and the effective nonlinear constant: $g + g_1 + g_2 \int K_1(z') dz'$. For $\omega_\perp = 100$, a few configuration have $\mu$ negative. A imaginary sound velocity is related to modulationally instability, thus those cases are ignored. The configurations on Table 6.2 have the nonlinear constant to be much lower, thus the organization is not in increasing order of the value $\mu$, but followed the same organization as the configurations shown in Table 6.1.

In the following simulations, the impurity moves at different speeds, varying from 0.1 to 1.4, as well as having different amplitudes $A$, ranging from 0.1 to 0.3. The following results are based on simulation in the absence of the harmonic external potential, that is $\omega_z = 0$. We run the time integration until the impurity leaves the domain, which is naturally large due to the boundary conditions.

The linear approximation of the critical velocity is shown in Fig. 6.9 for the first three configurations with $\omega_\perp = 2$. The same figure shows the numerical results for a subset of numerical simulations. For the two different amplitudes of the impurity and six different
velocities of the impurity, we searched for dark soliton nucleation in three simulations under the same parameter configuration. If nucleation is detected among the three simulations, we determined that nucleation appears as the given impurity velocity. Notice that for an impurity with an amplitude of \( A = 0.2 \) and moving at \( v = 0.5 \), nucleation was not detected for \( g_1 = -3 \) and \( g_2 = 5/\pi \). The critical velocity was estimated to \( v_c \approx 0.4731 \). For the first set of configurations with \( \omega_\perp = 2 \), the nucleation does not match linear approximation when the strength of the impurity is large. Nucleation should be detected if the velocity of the impurity is above the linear approximation according to the short-range approach. Nucleation of dark solitons where the value of the trapping frequency in the transverse direction is low required higher impurity velocities. For the simulations of \( \omega_\perp = 100 \), the results obtain were very good compared to the linear approximation.

Figure 6.8. The dotted (blue) line represents the line \( y = -x \int K_1(z') dz' \). The dot markers represent the different configurations used in the numerical runs.
Table 6.1. Table of different configuration settings with constant background of 1, and $\omega_\perp = 2$

<table>
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<th>Conf.</th>
<th>$g_1$</th>
<th>$g_2 \cdot \frac{\pi}{5}$</th>
<th>$\mu$</th>
<th>$v_s$</th>
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</thead>
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<td>0.638950356</td>
</tr>
<tr>
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<td>-3</td>
<td>1</td>
<td>0.591742443</td>
<td>0.769247972</td>
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<tr>
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<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
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<td>1.186700281</td>
</tr>
<tr>
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<td>0</td>
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Table 6.2. Table of different configuration settings with constant background of 1, and $\omega_\perp = 100$

<table>
<thead>
<tr>
<th>Conf.</th>
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<th>$g_2$</th>
<th>$\mu$</th>
<th>$v_s$</th>
</tr>
</thead>
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6.5 **Analytical Result**

Here we give a brief analysis to the dimensional reduction in the case that we consider only a nondipolar GP equation with an effective nonlinearity given by the

$$G = g_1 + g_2 \int K_1(z') \, dz', \text{ and } \int K_1(z') \, dz' = \frac{2\sqrt{2} \sqrt{\omega_\perp}}{\sqrt{\pi}}.$$  

The speed of sound depends only on $\mu = \rho G$:

$$v_s = \sqrt{\mu},$$

the critical velocity satisfies

$$v_c \approx \sqrt{\mu} - 2^\frac{3}{2} \frac{3\mu^\frac{1}{2}}{4} (\beta)^\frac{3}{2} \quad \beta \ll 1,$$  (6.3a)
Figure 6.9. The results of simulations for $\omega_\perp = 2$ for the first three configurations: $(g_1, \pi/5g_2)$: $(4, -1), (-3, 1), (1, 0)$ are shown in black red and blue, respectively. The curves shown in solid lines represent the analytical prediction of critical velocity for those configurations, Eq. (5.16). The speed of sound for each configuration are shown as horizontal lines. Each of the 36 points represents the results of three simulations with similar results. A star point represents simulations where nucleation was detected, and a empty circle corresponds to simulations where no dark soliton was detected. As the strength of the impurity increases, the nucleation of dipolar condensates does not agree with the short-range approximation.

and

$$v_c \approx \frac{\mu}{2\beta} \quad \beta \gg 1$$

(6.3b)

Thus, using the one-dimensional mean-field reduction of Section 2.2

$$g_1 = \frac{g_1 \omega_\perp}{2\pi} [1 + \frac{\epsilon_{dd}(1 - 3n_z^2)}{2}],$$

$$g_2 = \frac{3g_1 \epsilon_{dd} \sqrt{\omega_\perp}}{8\sqrt{2\pi}} (1 - 3n_z^2),$$

(6.4)

where $\epsilon_{dd} = \frac{4\pi g_2}{3g_1}$, is the ratio of the nonlinear constants of the full three dimensional system: $g_1$ and $g_2$. If $n_z = 0$, $G = \frac{g_1 \omega_\perp}{2\pi} (1 + 2\epsilon_{dd})$. For $n_z = \pm 1$, where the dipole direction is aligned with the longitudinal axis of the BEC, we have: $G = \frac{g_1 \omega_\perp}{2\pi} (1 - 4\epsilon_{dd})$. Therefore, the ratio $\epsilon_{dd}$ would change the effective nonlinearity constant. The ratio $\frac{\omega_z}{2\pi}$ is due to Gaussian profile of the ground state in the transverse direction.
CHAPTER 7
CONCLUSIONS AND FUTURE WORK

In this thesis, we explored the nucleation of dark solitons in the one-dimensional dipolar GP equation:

\[ i \frac{\partial u}{\partial t} = -\frac{1}{2} \partial_{zz} u + V_{1D} u + g_1 |u|^2 u + g_2 \left[ K_1 * |u|^2 \right] u, \]  

(7.1)

where the nonlinearity has a competitive behavior: \( g_1 g_2 < 0 \). Here, \( V_{1D} \) has a harmonic component \( \frac{\omega^2}{2} z^2 \), a moving localized Gaussian-shaped impurity. The nucleation of dark solitons occurs for velocities of the impurity above a critical value below the speed of sound. The critical velocity depends on the nonlinearities and the height of the background. The calculation of the convolution term \( [K_1 * |u|^2] = \int K_1(z - z') |u(z')|^2 dz' \) proves to be a challenge if not done in the Fourier space. If one uses the direct Newton method to find steady states for example, the Jacobian matrix is a full matrix. We discussed the use of numerical algorithms that facilitate the work of solving nonlinear equations, as well as the application of a time-split algorithm that benefits from the efficiency of FFT to perform time-simulations.

The one-dimensional model above was obtained by a dimensional reduction of the three-dimensional dipolar GP equation, where the trap strength in the longitudinal direction is weaker compared to the strength in the transverse direction. The separation of variables yields that the nonlinearity constants, \( g_1 \) and \( g_2 \), depend on the transverse trap strength \( \omega_\perp \), and the component of the dipole direction along the longitudinal direction \( n_z \). The kernel of the nonlocal term has been approximated by:

\[ K_1(z) = \omega_\perp k^3 \left( \frac{z^2 \omega_\perp}{2} + k^2 \right)^{-\frac{3}{2}}. \]  

(7.2)

As \( \omega_\perp \) increases, the dipolar kernel is more localized and the convolution behaves like a linear operator. The effective nonlinear constant is then \( G = g_1 + g_2 \int K_1(z') dz' \).

We proved analytically the conservation of mass and energy for the one-dimensional model; this was corroborated by numerical simulations for different configurations with competing nonlinearities. We also studied the modulational instability for homogeneous stationary states by finding the Bogoliubov-de Gennes equations in Fourier space; this is where the convolution is more tractable. We determined the modulational gain function that determines the exponential growth of perturbations of the homogeneous steady state of the
dipolar GP equation for a generic nonlocal interaction. For the one-dimensional dipolar kernel we determined the region \((g_1, g_2)\) in parameter space where homogeneous densities are modulationally stable. We found that when \(\omega_\perp\) is large, the line given by \(y = -x (\int K_1(z) \, dz)\) approximates well to the bifurcation line where the change of modulational stability occurs.

The exponential growth of the perturbation in the region of instability was confirmed for a small set of parameter values. In the case of modulational stability, the frequency of a homogeneous dipolar condensate of background density, \(\rho\), is approximated by the associated frequency \(\mu = G\rho\).

To solve the steady state for different trap configurations, we rely on the Newton-Krylov method, which was very effective in the parameter region close to instability. The nonlinear equation solver \texttt{nsol1} does not construct the full Jacobian matrix, but solves the linear system to find the Newton step. It is known that the Fourier transform of the convolution between two input functions, such as the density and the dipolar kernel, is the point product of the Fourier transform of the input functions. Fourier spectral methods rely on crossing back and forth between the physical space and the Fourier space. We can then use a pseudo spectral time-split algorithm that calculates the Laplacian operator in Fourier space in a much faster way. The composition of second-order methods is easy to implement to obtain a high order accuracy algorithm. This composition method is quite effective and fast for simulations where the presence of the external trap guarantees a periodic boundary condition.

Our main purpose was to find a critical velocity at which dark solitons nucleate and consider the effects of the nonlinear constants. This was done by solving the stability, in a co-moving reference, of a homogeneous background condensate. The approximation works well when the strength of the trap in the transverse direction is large, \(1 \ll \omega_\perp\). In such cases the dipolar kernel can be approximated by a \(\delta\)-function. For a fixed background density, the one-dimensional reduction dipolar BEC with competitive nonlinearities \(\epsilon_{dd} < 0\), the speed of sound, and therefore the critical velocity, is higher in the case that the impurity moves parallel to the dipole direction.

We numerically simulated the nucleation of dark solitons by adiabatically increasing the speed of a Gaussian impurity that moves across the condensate. We found agreement between the short-range approximation of the impurity and the numerical detection for large values of \(\omega_\perp\). In the case that \(\omega_\perp\) is small, the short-range approximation fails. However, it
should be possible to use the nonlinear Newton solver to do a similar procedure and obtain the critical velocity for a full dipolar GP equation.

Calculating the convolution in higher dimensions is quite challenging and simulations of the dipolar GP equation would be a very computationally-intensive process since the convolution must be done several times for each time step. Recent software and hardware developments in Graphics processing unit (GPU) cards allow for the acceleration of numerical simulations. For instance, NVIDIA manufactures GPU cards with parallel capabilities, well suited for simulations with double precision. Even though the GPU programming is a low level machine language, the platform to program the NVIDIA GPU cards, known as CUDA is accessible as an extension of programming language such as C, C++ and FORTRAN. The numerical codes can be written in C/C++ and compiled using nvcc, NVIDIA’s C/C++ compiler. The executable files can be wrapped and called from other programs, allowing user to run simulations from more user-friendly interface environments like MATLAB. In addition, CUDA has a library called cuFFT, which provides an interface to calculate the FFT up to 10 times faster than serial environments without having to write the FFT for the parallel environment inside the GPU cards.

In this thesis, we explored the critical velocity in one-dimensional dipolar condensates, and found the relation between the nonlinearity constants and the critical velocity. Since the dipolar kernel is anisotropic in higher dimensions, we expect that the critical velocity may be different if the impurity moves parallel or perpendicular to the dipole direction. We would like to develop a dipolar GP model for higher dimensional simulations. In a follow up future work, we will investigate numerically the dependence of the critical velocity if the impurity moves at an angle \( \theta \), and find the optimal angle for nucleation of vortices in two dimensions. Possible conceptual notions to address in the future would be to extend the one-dimensional analysis described in this thesis to the more challenging two-dimensional case.
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