

TEMPERATURE DEPENDENT DENSITY PROFILES AND COLLECTIVE OSCILLATIONS OF DIPOLAR DROPLETS

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We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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ABSTRACT

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Dipolar droplets are a novel form of Bose gas that form in a regime where the mean field theory predicts collapse. In the literature, the beyond mean field effects in the form of the Lee–Huang–Yang correction to the local chemical potential are used to explain the stability of these droplets. We employ the Hartree–Fock–Bogoliubov theory to include the beyond mean field terms in a systematic manner that also allows finite temperature calculations. In this thesis, we derive the modified Gross–Pitaevskii equation and the Bogoliubov–de Gennes equations, then solve the latter with a local density approximation and the former with a Gaussian variational ansatz. We show that Hartree–Fock–Bogoliubov theory reproduces the zero temperature results found in the literature, and indicates that the density profile and the collective oscillation of dipolar droplets depend on the temperature. We find that experimentally relevant temperatures ($T \sim 100\text{nK}$) may significantly alter the transition between low and high density phases, and change the collective oscillation frequencies of the system.

Keywords: Dipolar Droplets, Hartree–Fock–Bogoliubov Theory.

ÖZET

DİPOLAR DAMLACIKLARIN SICAKLIĞA BAĞLI YOĞUNLUK DAĞILIMI VE TOPLU SALINIMLARI

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Dipolar damlacıklar Bose gazının ortalama alan teorisinin çökme beklediği bir rejimde oluşan yeni bir halidir. Literatürde, bu damlacıkların kararlılığını göstermek için ortalama alanın ötesindeki etkiler, Lee–Huang–Yang düzeltmesi şeklinde kullanılmıştır. Biz Hartree–Fock–Bogoliubov teorisini kullanarak ortalama alanın ötesindeki etkileri sistematik bir şekilde hesaba katıp, şu ana kadar sadece sıfır sıcaklıkta çalışılan sistemin sonlu sıcaklardaki davranışını inceliyoruz. Bu tezde, Hartree–Fock–Bogoliubov teorisine değiştirilmiş Gross–Pitaevskii denklemini ve Bogoliubov–de Gennes denklemlerini türetilip, sonrakini yerel yoğunluk yaklaşımı (LDA) ve öncekini Gaussiyen varyasyonel anizats ile çözüyoruz. Hartree–Fock–Bogoliubov teorisinin literatürdeki sıfır sıcaklık denklemini yeniden türettiğini ve sıcaklığın yoğunluk profilini ve toplu salınımları etkilediğini gösteriyoruz. Deneylerde karşılaşılan sıcaklıkların düşük yoğunluklu fazdan yüksek yoğunluklu faza geçişte önemli etkileri olabileceğini ve toplu salınım frekanslarını ciddi bir şekilde değiştirebileceğini buluyoruz.

Anahtar sözcükler: Dipolar Damlacıklar, Hartree–Fock–Bogoliubov Teorisi.

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Chapter 1

Introduction

Bose–Einstein condensation is one of the biggest achievements of modern physics, from its theoretical proposition [1, 2] to its experimental observation [3, 4]. Bosons, whole-spin particles, have the symmetry property that allows them to have same quantum wavefunction. Therefore, at low temperatures, a system of bosons is expected to condense in a way that all particles occupy the same state (in other words, have the same wavefunction). Continual efforts of high-level research resulted in the experimental observation(s) of Bose–Einstein condensation in optically trapped ultracold atoms seventy years after its prediction [3, 4].

In ultracold atom experiments effective Hamiltonian of the system has two parts. The first part is the single particle Hamiltonian, which is comprised of kinetic energy and trapping potential energy. The second part is the interaction Hamiltonian where the interaction is usually the contact interaction between atoms. Methodically prepared in a certain quantum (hyperfine) state, the atoms normally interact via a single channel, where this interaction can be tuned with the help of Feshbach resonances [5]. This allows the interaction potential to be modeled by a delta function with a tunable amplitude given in terms of the s -wave scattering length. These trapped atoms may also have a magnetic dipole moment determined by their electronic configuration [6]. Therefore, in systems with considerable dipolar interaction, the interaction Hamiltonian contains both

the short range (contact) and the long range (dipole-dipole) interaction, where often the dipoles are aligned with an external magnetic field. Dipolar interaction is anisotropic where the interaction is governed not only by the distance between atoms, but also by the alignment of the two dipole moments. Moreover, its anisotropy is such that the interaction may be attractive or repulsive depending on the configuration of the two dipoles.

For weakly interacting bosons, Gross and Pitaevskii have derived an equation, that describes the condensate wavefunction within the aforementioned description [7]. Gross–Pitaevskii mean field theory remained valid for a long time for ultra cold atom experiments. In 2015, however, the Stuttgart group led by Tilman Pfau reported the observation dipolar droplets, which exist in a parameter regime where the mean field theory predicts collapse [8].

Systems, for which the dipolar interaction is dominant over the contact repulsion, are expected to collapse since two dipoles arranged in the head-to-tail configuration attract and come together overcoming the contact repulsion. Nevertheless, a formation of stable condensates is observed for dysprosium atoms whose scattering length is reduced below a dipolar interaction scattering length [8]. This condensate was labeled: "dipolar droplet", echoing the two component droplets¹. The Stuttgart group later reported that these droplets are indeed a condensed state of matter having the same phase [11], and the droplets can form without an external trapping potential [12]. In 2016, Innsbruck group led by Francesca Ferlaino showed droplet formation in another magnetic atom, erbium [13].

Not conforming to mean field theory, these droplets are explained by beyond mean field effects. It is demonstrated that the beyond mean field corrections may explain the droplet formation and calculate the density to the correct order of magnitude observed in experiments [11]. In the mean field approximation, total interaction energy scales with the-condensate-density-squared with a coefficient that depends on the specifics of the interaction potential. If the coefficient is

¹It is called droplet as it does not require an external trapping potential [9]. Two component droplets have been observed by Barcelona group led by Leticia Tarruell [10].

negative (as in the droplet experiments), the system tends to increase the density without a bound leading to a collapse. Beyond mean field correction (Lee–Huang–Yang correction) to total interaction energy scales with the condensate density to power $5/2$ with a coefficient that is always positive. Hence, it results in a finite value for the condensate density and arrests the collapse.

Although the Lee–Huang–Yang correction, is a correction to the total energy, in the current literature it is patched onto the Gross–Pitaevskii equation describing the condensate wavefunction. This treatment is borrowed from the work of Dmitry Petrov on two component Bose gases, where a special stability condition is studied with regard to interaction strengths (inter- and intra- species) [9]. For dipolar droplets, the Hannover group led by Luis Santos and the Otago group led by Blair Blakie were the first to employ the modified Gross–Pitaevskii equation, and concurrently reported the stability of the droplets as a function of the relative dipolar strength and the trap aspect ratio [14, 15, 16].

We believe the introduction of the correction term in the Gross–Pitaevskii equation is not transparent about the assumptions made in the calculation. The Hartree–Fock–Bogoliubov theory is developed to handle beyond mean field (fluctuation) effects [17, 18]. Treating the fluctuation operators with the Hartree–Fock–Bogoliubov theory, we derive the modified Gross–Pitaevskii equation. The correction terms we derive are compatible with the Lee–Huang–Yang correction term used in the literature. Moreover, it is expressed in terms of the non-condensate densities, which provide a better understanding of the system, and can be calculated at non-zero temperatures.

The non-condensate densities are a result of quantum fluctuations and thermal excitations in the system. Excitation spectrum of the condensate is given by the Bogoliubov–de Gennes equations [19], a set of coupled differential equations requiring prior knowledge of the condensate wavefunction. Therefore, exact solution of these equations requires a self-consistent numerical procedure involving a non-linear equation as well as three dimensional Schrödinger-like coupled equations. Hence, to gain an insight of the effects of thermal fluctuations as well as quantum fluctuations on the system, we employ certain of approximation methods. The

first method is the semi-classical approximation for the Bogoliubov amplitudes. Together with a local density approximation for the condensate wavefunction, we calculate the correction terms as a function of not only the condensate density and the relative dipolar interaction strength but also temperature. One of the problems in calculating these terms is the collapsing modes at large wavelengths. These modes are a byproduct of the approximations used, and can be eliminated by a suitable cutoff which excludes the modes with wavelengths longer than a characteristic length of the condensate. Semi-classical approximation being better suited for the short wavelength modes further justifies such a cutoff. Although this procedure involves a somewhat arbitrary choice of cutoff wavelength, it results in a correction term which is of the correct order of magnitude. Second problem is the temperature dependence being not so straightforward to deal with because of the convoluted Bose–Einstein distribution function. We solve this with a second order which still allows for a thermal correction within the confidence levels of all the approximations made.

With the temperature dependent correction terms added, the modified Gross–Pitaevskii equation can be solved for the condensate wavefunction. One route is the full numerical solution for the equation, which will grant a precise wavefunction albeit limited by the approximations. The other route to estimate the effects of the correction terms on the condensate wavefunction is employing a Gaussian variational ansatz. Scanning the parameter space of the condensate widths for the Gaussian ansatz, we find the minimum of the energy functional corresponding to the modified Gross–Pitaevskii equation. Additionally, using the total energy functional, we write the corresponding Lagrangian density for the wavefunction. Then, we study the equation of motion for the condensate widths derived from the Lagrangian of the system, hence the collective oscillation frequencies of the system.

We focus on two systems of dipolar droplets that replicate the experimental conditions in dysprosium [8] and erbium [13] experiments. Both systems clearly show that the shape of the condensate wavefunction and collective oscillation frequencies depend on the temperature.

Chapter 2

The Hamiltonian

The second quantized Hamiltonian for the interacting many body system is:

$$\begin{aligned} \hat{H} = & \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2M} + U_{\text{tr}}(\mathbf{x}) \right) \hat{\psi}(\mathbf{x}) \\ & + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x}), \end{aligned} \quad (2.1)$$

where $\hat{\psi}^\dagger(\mathbf{x})$ and $\hat{\psi}(\mathbf{x})$ are creation and annihilation operators, respectively, satisfying the commutation relation $[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}')$. M is the mass of the bosons, $U_{\text{tr}}(\mathbf{x})$ is the trapping potential, and $V_{\text{int}}(\mathbf{r})$ is the interaction potential between bosons. In this thesis, the interaction potential is comprised of the short range repulsion $V_{\text{short}}(\mathbf{r}) = g\delta(\mathbf{r})$ with $g = \frac{4\pi\hbar^2 a_s}{M}$, where a_s is the s-wave scattering length; and the dipole-dipole interaction $V_{\text{long}}(\mathbf{r}) = \frac{\mu_0\mu^2}{4\pi} \frac{1-3\cos^2\theta_{\mathbf{r}}}{|\mathbf{r}|^3}$, where μ is the dipole moment polarized along z axis, and $\theta_{\mathbf{r}}$ is the angle between \mathbf{r} and the z axis. Instead of using s-wave scattering length and dipole moments separately, we define $\epsilon_{dd} = a_{dd}/a_s$ where a_{dd} is the dipolar length given by $a_{dd} = M\mu_0\mu^2/12\pi\hbar^2$. Then, the interaction potential becomes: $V_{\text{int}}(\mathbf{r}) = g \left(\delta(\mathbf{r}) + \frac{3\epsilon_{dd}}{4\pi} \frac{1-3\cos^2\theta_{\mathbf{r}}}{|\mathbf{r}|^3} \right)$.

Second quantized field operator can be expressed as: $\hat{\psi}(\mathbf{x}) = \sum_n \psi_n(\mathbf{x}) \hat{a}_n$, where $\{\psi_n(\mathbf{x})\}$ is a complete and orthonormal set of functions, and \hat{a}_n (\hat{a}_n^\dagger) is annihilation (creation) operator for n th state. In the case of Bose–Einstein condensation, a single particle state is occupied by a large fraction of total particles

(in the eigenbasis of the density matrix), therefore the field operator can be split into condensate and non-condensate parts: $\hat{\psi}(\mathbf{x}) = \psi_0(\mathbf{x})\hat{a}_0 + \hat{\phi}(\mathbf{x})$. $\hat{\phi}(\mathbf{x})$, called the fluctuation operator. The fluctuation satisfies the commutation relation $[\hat{\phi}(\mathbf{x}), \hat{\phi}^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}') - \psi_0(\mathbf{x})\psi_0^*(\mathbf{x}')$.

Assuming $N - \bar{n}_0 \ll N$, where $\bar{n}_0 = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle$ is the number of particles in the condensate state, we notice $[\hat{a}_0, \hat{a}_0^\dagger] = 1 \ll \bar{n}_0$. Therefore the action of the condensate operator on the many body wavefunction can be approximated by identity operator, $\hat{a}_0, \hat{a}_0^\dagger \rightarrow \sqrt{\bar{n}_0}\mathbb{1} \approx \sqrt{N}\mathbb{1}$. Defining the function $\Psi(\mathbf{x}) = \sqrt{N}\psi_0(\mathbf{x})$, which satisfies $\int d^3\mathbf{x}\Psi^*(\mathbf{x})\Psi(\mathbf{x}) = N$, we write the field operator as $\hat{\psi}(\mathbf{x}) = \Psi(\mathbf{x}) + \hat{\phi}(\mathbf{x})$.

This prescription violates the particle number conserving nature of the Hamiltonian. Hence, the grand canonical Hamiltonian must be used $\hat{H} \rightarrow \hat{H} - \mu\hat{N}$, where \hat{N} is the total particle number operator $\hat{N} = \int d^3\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$, and μ is the chemical potential. The Hamiltonian can be expanded in orders of fluctuation operators $\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4$, where

$$\begin{aligned} \hat{H}_0 = & \int d^3\mathbf{x}\Psi^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) \Psi(\mathbf{x}) \\ & + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x} - \mathbf{x}')\Psi(\mathbf{x}')\Psi(\mathbf{x}), \end{aligned} \quad (2.2)$$

$$\begin{aligned} \hat{H}_1 = & \int d^3\mathbf{x}\Psi^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) \hat{\phi}(\mathbf{x}) \\ & + \int d^3\mathbf{x}\hat{\phi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) \Psi(\mathbf{x}) \\ & + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\hat{\phi}^\dagger(\mathbf{x})\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x} - \mathbf{x}')\Psi(\mathbf{x}')\Psi(\mathbf{x}) \\ & + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})\hat{\phi}^\dagger(\mathbf{x}')V_{\text{int}}(\mathbf{x} - \mathbf{x}')\Psi(\mathbf{x}')\Psi(\mathbf{x}) \\ & + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x} - \mathbf{x}')\hat{\phi}(\mathbf{x}')\Psi(\mathbf{x}) \\ & + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x} - \mathbf{x}')\Psi(\mathbf{x}')\hat{\phi}(\mathbf{x}), \end{aligned} \quad (2.3)$$

$$\begin{aligned}
\hat{H}_2 = & \int d^3\mathbf{x} \hat{\phi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}), \tag{2.4}
\end{aligned}$$

$$\begin{aligned}
\hat{H}_3 = & \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \Psi(\mathbf{x}), \tag{2.5}
\end{aligned}$$

and

$$\hat{H}_4 = \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \hat{\phi}^\dagger(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \hat{\phi}(\mathbf{x}') \hat{\phi}(\mathbf{x}). \tag{2.6}$$

In this thesis, we will derive the modified Gross–Pitaevskii equation from \hat{H}_1 and \hat{H}_3 , and the Bogoliubov–de Gennes equations from \hat{H}_2 .

Chapter 3

Modified Gross–Pitaevskii Equation

Once the Hamiltonian is expressed in orders of fluctuation operator, we notice that terms have the order of magnitudes: N^2 , $N^{3/2}$, N , \sqrt{N} and 1. Therefore, to diagonalize the Hamiltonian, one neglects the third and fourth order terms (\hat{H}_3, \hat{H}_4). Of the remaining terms, \hat{H}_0 is the ground state energy of the system. \hat{H}_1 involves the first order terms in fluctuation operator, which must vanish in the ground state. With this observation, the equation for the condensate wavefunction (Ψ) is obtained from \hat{H}_1 [7]. Finally, \hat{H}_2 is diagonalized using Bogoliubov transformation (see the section on Bogoliubov–de Gennes equations).

A way to improve this treatment is to include terms of higher orders. This can be done via the Hartree–Fock factorization. It states the operator $\hat{x}\hat{y}\hat{z}$ can be approximated by [17]

$$\hat{x}\hat{y}\hat{z} \approx \langle \hat{y}\hat{z} \rangle \hat{x} + \langle \hat{x}\hat{z} \rangle \hat{y} + \langle \hat{x}\hat{y} \rangle \hat{z}. \quad (3.1)$$

Applying this treatment to \hat{H}_3 yields:

$$\begin{aligned}
\hat{H}_3 \approx & \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}(\mathbf{x}')\hat{\phi}(\mathbf{x})\rangle\hat{\phi}^\dagger(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}(\mathbf{x}')\hat{\phi}(\mathbf{x})\rangle\hat{\phi}^\dagger(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x}')\hat{\phi}(\mathbf{x})\rangle\hat{\phi}^\dagger(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x}')\hat{\phi}(\mathbf{x}')\rangle\hat{\phi}^\dagger(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x}')\hat{\phi}(\mathbf{x})\rangle\hat{\phi}(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x})\rangle\hat{\phi}(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x})\rangle\hat{\phi}^\dagger(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x}')\rangle\hat{\phi}^\dagger(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x}')\hat{\phi}(\mathbf{x}')\rangle\hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x}')\rangle\hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}^\dagger(\mathbf{x}')\rangle\hat{\phi}(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}^\dagger(\mathbf{x}')\rangle\hat{\phi}(\mathbf{x}'). \tag{3.2}
\end{aligned}$$

Here, the non-condensate densities are introduced

$$\tilde{n}(\mathbf{x}, \mathbf{x}') = \langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x}')\rangle, \tag{3.3}$$

$$\tilde{n}(\mathbf{x}) = \langle\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x})\rangle, \tag{3.4}$$

$$\tilde{m}(\mathbf{x}, \mathbf{x}') = \langle\hat{\phi}(\mathbf{x})\hat{\phi}(\mathbf{x}')\rangle, \tag{3.5}$$

where \tilde{n} is the direct non-condensate density, and \tilde{m} is the anomalous non-condensate density. Hence, the first and the third order Hamiltonians can be

combined, and the term that includes $\hat{\phi}^\dagger$ can be written as:

$$\begin{aligned}
\hat{H}_{1\&3\rightarrow 1}\{\hat{\phi}^\dagger(\mathbf{x})\} &= \int d^3\mathbf{x}\hat{\phi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2\nabla^2}{2M}-\mu+U_{\text{tr}}(\mathbf{x})\right)\Psi(\mathbf{x}) \\
&+ \iint d^3\mathbf{x}d^3\mathbf{x}'\hat{\phi}^\dagger(\mathbf{x})\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}')\Psi(\mathbf{x}) \\
&+ \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\tilde{m}(\mathbf{x}',\mathbf{x})\hat{\phi}^\dagger(\mathbf{x}) \\
&+ \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\tilde{n}(\mathbf{x}',\mathbf{x})\hat{\phi}^\dagger(\mathbf{x}) \\
&+ \iint d^3\mathbf{x}d^3\mathbf{x}'\Psi(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\tilde{n}(\mathbf{x}',\mathbf{x})\hat{\phi}^\dagger(\mathbf{x}). \tag{3.6}
\end{aligned}$$

Note that the 1/2 fractions disappeared because of the $\mathbf{x} \leftrightarrow \mathbf{x}'$ symmetry of the terms.

Since the first order terms in fluctuations in the Hamiltonian must vanish.

$$\begin{aligned}
&\left[-\frac{\hbar^2\nabla^2}{2M}-\mu+U_{\text{tr}}(\mathbf{x})+\int d^3\mathbf{x}'V_{\text{int}}(\mathbf{x}-\mathbf{x}')|\Psi(\mathbf{x}')|^2\right]\Psi(\mathbf{x}) \\
&+ \left(\int d^3\mathbf{x}'V_{\text{int}}(\mathbf{x}-\mathbf{x}')\tilde{n}(\mathbf{x}')\right)\Psi(\mathbf{x}) \\
&+ \int d^3\mathbf{x}'\tilde{n}(\mathbf{x}',\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}') \\
&+ \int d^3\mathbf{x}'\tilde{m}(\mathbf{x}',\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi^*(\mathbf{x}') = 0. \tag{3.7}
\end{aligned}$$

This is the Gross–Pitaevskii equation modified by the correction terms arising from the non-condensate densities. At zero temperature this equation is equivalent to what is being used in the literature where the correction term is the Lee–Huang–Yang energy [14, 15, 16]. Hartree–Fock–Bogoliubov theory allows for non zero temperature calculations of the system as the non-condensate densities are linked to quasi particle excitations.

3.1 Correction terms

The modified Gross–Pitaevskii equation contains three correction terms. The first one is the Hartree potential due to non-condensate atoms:

$$\Phi_1(\mathbf{x}) = \int d^3\mathbf{x}' V_{\text{int}}(\mathbf{x} - \mathbf{x}') \tilde{n}(\mathbf{x}'). \quad (3.8)$$

This term is absent in the current literature involving the Lee–Huang–Yang correction.

The second and third correction terms are Ω_n and Ω_m , which are defined as:

$$\Omega_n(\mathbf{x})\Psi(\mathbf{x}) = \int d^3\mathbf{x}' \tilde{n}(\mathbf{x}', \mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}'), \quad (3.9)$$

and

$$\Omega_m(\mathbf{x})\Psi(\mathbf{x}) = \int d^3\mathbf{x}' \tilde{m}(\mathbf{x}', \mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}'). \quad (3.10)$$

In the following chapters, we show that $\Omega_n(\mathbf{x}) + \Omega_m(\mathbf{x})$ is equivalent to the Lee–Huang–Yang correction $\Delta\mu(\mathbf{x})$ found in the literature. To calculate the correction terms which depend on the non-condensate densities, we derive the governing equations for excitations called Bogoliubov–de Gennes equations in the next chapter.

Chapter 4

Bogoliubov–de Gennes Equations

Excitation spectrum is obtained by the diagonalization of the second order terms in fluctuations. In an interacting boson system, the ground state can be described as a large number of particles occupying the condensate state but with some particles filling non-condensate states even at zero temperature. This is called quantum fluctuations. Since the number of particles in the condensate state is saturated, not only removing a particle from the condensate state results in an excitation, but also putting a particle into the condensate state does result in an excitation. Therefore, a single (quasi) particle excitation operator can be outlined as a linear combination of the two fluctuation operators: $\hat{\alpha} = \int (\dots \hat{\phi} + \dots \hat{\phi}^\dagger)$. Hence, the fluctuation operators can be expressed in terms of quasi particle excitation operators,

$$\hat{\phi}(\mathbf{x}) = \sum_j \left(u_j(\mathbf{x}) \hat{\alpha}_j - v_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger \right) \quad (4.1)$$

$$\hat{\phi}^\dagger(\mathbf{x}) = \sum_j \left(u_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger - v_j(\mathbf{x}) \hat{\alpha}_j \right), \quad (4.2)$$

where $\{u_j(\mathbf{x}), v_j(\mathbf{x})\}$ are Bogoliubov amplitudes, and the quasi particle operators obey the usual commutation relations: $[\hat{\alpha}_j, \hat{\alpha}_k] = [\hat{\alpha}_j^\dagger, \hat{\alpha}_k^\dagger] = 0$ and $[\hat{\alpha}_j, \hat{\alpha}_k^\dagger] = \delta_{j,k}$.

With this transformation, called the Bogoliubov transformation, \hat{H}_2 becomes:

$$\begin{aligned}
\hat{H}_2 = & \sum_{j,k} \int d^3\mathbf{x} \left(u_j^*(\mathbf{x})\hat{\alpha}_j^\dagger - v_j(\mathbf{x})\hat{\alpha}_j \right) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) \left(u_k(\mathbf{x})\hat{\alpha}_k - v_k^*(\mathbf{x})\hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}' \left(u_j^*(\mathbf{x})\hat{\alpha}_j^\dagger - v_j(\mathbf{x})\hat{\alpha}_j \right) \Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}') \left(u_k(\mathbf{x})\hat{\alpha}_k - v_k^*(\mathbf{x})\hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}' \Psi^*(\mathbf{x}) \left(u_j^*(\mathbf{x}')\hat{\alpha}_j^\dagger - v_j(\mathbf{x}')\hat{\alpha}_j \right) V_{\text{int}}(\mathbf{x}-\mathbf{x}') \left(u_k(\mathbf{x}')\hat{\alpha}_k - v_k^*(\mathbf{x}')\hat{\alpha}_k^\dagger \right) \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}' \left(u_j^*(\mathbf{x})\hat{\alpha}_j^\dagger - v_j(\mathbf{x})\hat{\alpha}_j \right) \Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}') \left(u_k(\mathbf{x}')\hat{\alpha}_k - v_k^*(\mathbf{x}')\hat{\alpha}_k^\dagger \right) \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}' \Psi^*(\mathbf{x}) \left(u_j^*(\mathbf{x}')\hat{\alpha}_j^\dagger - v_j(\mathbf{x}')\hat{\alpha}_j \right) V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}') \left(u_k(\mathbf{x})\hat{\alpha}_k - v_k^*(\mathbf{x})\hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}' \Psi^*(\mathbf{x})\Psi^*(\mathbf{x}')V_{\text{int}}(\mathbf{x}-\mathbf{x}') \left(u_j(\mathbf{x}')\hat{\alpha}_j - v_j^*(\mathbf{x}')\hat{\alpha}_j^\dagger \right) \left(u_k(\mathbf{x})\hat{\alpha}_k - v_k^*(\mathbf{x})\hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x}d^3\mathbf{x}' \left(u_j^*(\mathbf{x})\hat{\alpha}_j^\dagger - v_j(\mathbf{x})\hat{\alpha}_j \right) \left(u_k^*(\mathbf{x}')\hat{\alpha}_k^\dagger - v_k(\mathbf{x}')\hat{\alpha}_k \right) V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}')\Psi(\mathbf{x}).
\end{aligned} \tag{4.3}$$

If the Bogoliubov amplitudes satisfy the following coupled differential equations called the Bogoliubov–de Gennes equations [19]:

$$\begin{aligned}
\left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u_j(\mathbf{x}) + \int d^3\mathbf{x}' \Psi(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi^*(\mathbf{x}')u_j(\mathbf{x}') \\
- \int d^3\mathbf{x}' \Psi(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}')v_j(\mathbf{x}') = E_j u_j(\mathbf{x}), \tag{4.4}
\end{aligned}$$

$$\begin{aligned}
\left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) v_j(\mathbf{x}) + \int d^3\mathbf{x}' \Psi^*(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi(\mathbf{x}')v_j(\mathbf{x}') \\
- \int d^3\mathbf{x}' \Psi^*(\mathbf{x})V_{\text{int}}(\mathbf{x}-\mathbf{x}')\Psi^*(\mathbf{x}')u_j(\mathbf{x}') = -E_j v_j(\mathbf{x}), \tag{4.5}
\end{aligned}$$

the Hamiltonian becomes,

$$\begin{aligned}
\hat{H}_2 = & \sum_{j,k} \frac{1}{2} \int d^3\mathbf{x} u_j^*(\mathbf{x}) u_k(\mathbf{x}) (E_j^* + E_k) (\hat{\alpha}_j^\dagger \hat{\alpha}_k) \\
& - \frac{1}{2} \int d^3\mathbf{x} v_j(\mathbf{x}) v_k^*(\mathbf{x}) (E_j + E_k^*) (\hat{\alpha}_j \hat{\alpha}_k^\dagger) \\
& + \frac{1}{2} \int d^3\mathbf{x} v_j(\mathbf{x}) u_k(\mathbf{x}) (E_j - E_k) (\hat{\alpha}_j \hat{\alpha}_k) \\
& - \frac{1}{2} \int d^3\mathbf{x} u_j^*(\mathbf{x}) v_k^*(\mathbf{x}) (E_j^* - E_k^*) (\hat{\alpha}_j^\dagger \hat{\alpha}_k^\dagger). \tag{4.6}
\end{aligned}$$

Multiplying the Bogoliubov–de Gennes equations with the pairs $\{u_k^*(\mathbf{x}), v_k^*(\mathbf{x})\}$, $\{v_k(\mathbf{x}), u_k(\mathbf{x})\}$, and integrating over space yields

$$(E_j - E_k^*) \int d^3\mathbf{x} [u_j(\mathbf{x}) u_k^*(\mathbf{x}) - v_j(\mathbf{x}) v_k^*(\mathbf{x})] = 0, \tag{4.7}$$

$$(E_j + E_k) \int d^3\mathbf{x} [u_j(\mathbf{x}) v_k(\mathbf{x}) - v_j(\mathbf{x}) u_k(\mathbf{x})] = 0, \tag{4.8}$$

respectively. Since the normalization constant is nonzero, $j = k$ case indicates that E_j are real, and the normalization condition is

$$\int d^3\mathbf{x} [u_j(\mathbf{x}) u_k^*(\mathbf{x}) - v_j(\mathbf{x}) v_k^*(\mathbf{x})] = \delta_{j,k}. \tag{4.9}$$

Thus, the Hamiltonian is diagonalized in terms of the quasi particle excitation operators

$$\hat{H}_2 = \sum_j E_j \hat{\alpha}_j^\dagger \hat{\alpha}_j - \sum_j E_j \int d^3\mathbf{x} |v_j(\mathbf{x})|^2. \tag{4.10}$$

The excitation modes are decoupled, and can be viewed as free quasi particle excitations. Therefore, the population of each excitation mode is given by the Bose statistics

$$\langle \hat{\alpha}_j^\dagger \hat{\alpha}_k \rangle = \delta_{j,k} N_B(E_j), \tag{4.11}$$

$$\langle \hat{\alpha}_j^\dagger \hat{\alpha}_k^\dagger \rangle = \langle \hat{\alpha}_j \hat{\alpha}_k \rangle = 0, \tag{4.12}$$

where $N_B(E) = 1 / \left(\exp \left[\frac{E}{k_B T} \right] - 1 \right)$.

Previously defined non-condensate densities can be expressed in terms of Bogoliubov amplitudes:

$$\tilde{n}(\mathbf{x}', \mathbf{x}) = \sum_j (v_j(\mathbf{x}') v_j^*(\mathbf{x}) + N_B(E_j) [u_j^*(\mathbf{x}') u_j(\mathbf{x}) + v_j(\mathbf{x}') v_j^*(\mathbf{x})]), \tag{4.13}$$

$$\tilde{m}(\mathbf{x}', \mathbf{x}) = - \sum_j (u_j(\mathbf{x}')v_j^*(\mathbf{x}) + N_B(E_j) [v_j^*(\mathbf{x}')u_j(\mathbf{x}) + u_j(\mathbf{x}')v_j^*(\mathbf{x})]). \quad (4.14)$$

Although the modified Gross–Pitaevskii equation contains non-condensate densities, it is derived with a large condensate fraction assumption. Therefore, it is reliable at temperatures well below Bose–Einstein critical temperature. Nevertheless, there is another temperature scale (other than the critical temperature) at which the thermal depletion (the first term in Eq. 4.10) is comparable to the quantum depletion at zero temperature in interacting systems (the second term in Eq. 4.10). Therefore, the modified Gross–Pitaevskii equation is valid for this temperature range as it is valid for the zero temperature.

Chapter 5

Semi-Classical and Local Density Approximations

The Gross–Pitaevskii and the Bogoliubov-de Gennes equations represent a self consistent picture of the condensate and the excitations, as the modified Gross–Pitaevskii equation includes the non-condensate densities. To solve the Bogoliubov-de Gennes equations, the condensate wavefunction must be known. In an ideal case, these equations are solved numerically. However, an insight into the physics of the system can be obtained by solving the Bogoliubov-de Gennes equations with a semi-classical approximation for the Bogoliubov amplitudes and a local density approximation for the condensate wavefunction. With the assumption that the condensate density is a slowly varying function of position, we solve the Bogoliubov-de Gennes equations locally with substitution [20]

$$u_j(\mathbf{x}) \rightarrow u(\mathbf{x}, \mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}, \quad E_j \rightarrow E(\mathbf{x}, \mathbf{k}), \quad \sum_j \rightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3}, \quad (5.1)$$

where $u(\mathbf{x}, \mathbf{k})$ is also a slowly varying function of position, and $E(\mathbf{x}, \mathbf{k})$ is the continuous excitation spectrum. This substitution yield the new orthonormality

condition for the Bogoliubov amplitudes

$$\begin{aligned} \sum_k \int d^3\mathbf{x} [u_j(\mathbf{x})u_k^*(\mathbf{x}) - v_j(\mathbf{x})v_k^*(\mathbf{x})] &= 1 \\ \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \int d^3\mathbf{x} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} [u(\mathbf{x},\mathbf{k})u^*(\mathbf{x},\mathbf{k}') - v(\mathbf{x},\mathbf{k})v^*(\mathbf{x},\mathbf{k}')] &= 1 \\ |u(\mathbf{x},\mathbf{k})|^2 - |v(\mathbf{x},\mathbf{k})|^2 &= 1, \end{aligned} \quad (5.2)$$

where the term in the square brackets in the second row is thought to be constant as opposed to rapidly varying exponential term.

We note that within the local density approximation the chemical potential (excluding the non-condensate terms) is $\mu \approx U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x})$ (Thomas–Fermi approximation). Hence, we substitute the semi-classical Bogoliubov amplitudes in the Bogoliubov-de Gennes equations, and multiply these equations with $e^{-i\mathbf{k}\cdot\mathbf{x}}$ for convenience. The first term in these equations become

$$e^{-i\mathbf{k}\cdot\mathbf{x}} \left(-\frac{\hbar^2 \nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u(\mathbf{x},\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \approx \varepsilon_{\mathbf{k}} u(\mathbf{x},\mathbf{k}), \quad (5.3)$$

where $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2M}$. The terms including the following integral become

$$\begin{aligned} \Psi(\mathbf{x}) \int d^3\mathbf{x}' V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u(\mathbf{x}',\mathbf{k}) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\ = \Psi(\mathbf{x}) \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \int d^3\mathbf{x}' \tilde{V}_{\text{int}}(\mathbf{k}') \Psi(\mathbf{x}') u(\mathbf{x}',\mathbf{k}) e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{x}-\mathbf{x}')} \\ \approx n_0(\mathbf{x}) \tilde{V}_{\text{int}}(\mathbf{k}) u(\mathbf{x},\mathbf{k}), \end{aligned} \quad (5.4)$$

where $n_0(\mathbf{x}) = |\Psi(\mathbf{x})|^2$ (with the assumption that the condensate wavefunction is real). Therefore, the Bogoliubov–de Gennes equations simplify to the algebraic form:

$$\varepsilon_{\mathbf{k}} u(\mathbf{x},\mathbf{k}) + n_0(\mathbf{x}) \tilde{V}_{\text{int}}(\mathbf{k}) u(\mathbf{x},\mathbf{k}) - n_0(\mathbf{x}) \tilde{V}_{\text{int}}(\mathbf{k}) v(\mathbf{x},\mathbf{k}) = E(\mathbf{x},\mathbf{k}) u(\mathbf{x},\mathbf{k}), \quad (5.5)$$

$$\varepsilon_{\mathbf{k}} v(\mathbf{x},\mathbf{k}) + n_0(\mathbf{x}) \tilde{V}_{\text{int}}(\mathbf{k}) v(\mathbf{x},\mathbf{k}) - n_0(\mathbf{x}) \tilde{V}_{\text{int}}(\mathbf{k}) u(\mathbf{x},\mathbf{k}) = -E(\mathbf{x},\mathbf{k}) v(\mathbf{x},\mathbf{k}). \quad (5.6)$$

Then, the energy spectrum reads:

$$E(\mathbf{x},\mathbf{k}) = \sqrt{\varepsilon_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} + 2n_0(\mathbf{x}) \tilde{V}_{\text{int}}(\mathbf{k}) \right)}. \quad (5.7)$$

The energy spectrum given by the equation above contains modes with imaginary energy for long wavelengths when $\epsilon_{dd} > 1$. This is because the excitation spectrum is highly discrete for low energy excitations, which is not captured within the continuous spectrum. Moreover, for a finite size system the wavelengths of the low lying excitations is determined by the system size.

Therefore, we use an isotropic cut off, $k_c^{(I)} = \pi/2\xi$, which omits modes with longer wavelength than 4ξ , where ξ is the coherence length of the condensate given by $\xi = \hbar/\sqrt{2Mgn_0}$. In the literature, there are two other cut off choices: [16] uses an elliptical cut off, $k_c^{(II)}(\vartheta) = 1/\sqrt{\sin^2 \vartheta/k_{c,\rho}^2 + \cos^2 \vartheta/k_{c,z}^2}$; and [14] uses the cutoff, $k_c^{(III)}(\vartheta) = \sqrt{k_{c,\rho}^2 \sin^2 \vartheta + k_{c,z}^2 \cos^2 \vartheta}$, where $\{k_{c,\rho}, k_{c,z}\} = \{1.5, 0.25\}\xi^{-1}$.

Another method is to only take the real part into account. However, the density of states at zero energy for $\epsilon_{dd} > 1$ is finite, resulting in a divergence in non-zero temperature calculations. Our cut off choice also remedies this.

In Fig. 5.1, we plot these cutoff choices as well as the region of imaginary modes in the k-space. We see in Fig. 5.2 all of these cutoff choices yield similar results.

5.1 Correction terms within the local density approximation

The correction terms can be expressed within the same local density approximation:

$$\Omega_n(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) |v(\mathbf{x}, \mathbf{k})|^2 + \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) N_B(E(\mathbf{x}, \mathbf{k})) [|u(\mathbf{x}, \mathbf{k})|^2 + |v(\mathbf{x}, \mathbf{k})|^2], \quad (5.8)$$

$$\Omega_m(\mathbf{x}) = - \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) u(\mathbf{x}, \mathbf{k}) v^*(\mathbf{x}, \mathbf{k}) - \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) 2N_B(E(\mathbf{x}, \mathbf{k})) u(\mathbf{x}, \mathbf{k}) v^*(\mathbf{x}, \mathbf{k}), \quad (5.9)$$

where $\tilde{V}_{\text{int}}(\mathbf{k}) = g[1 + \epsilon_{dd}(3 \cos^2 \theta_{\mathbf{k}} - 1)]$ is the Fourier transform of the interaction potential ($\tilde{V}_{\text{int}}(\mathbf{k}) = \int d^3\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} V_{\text{int}}(\mathbf{x})$).

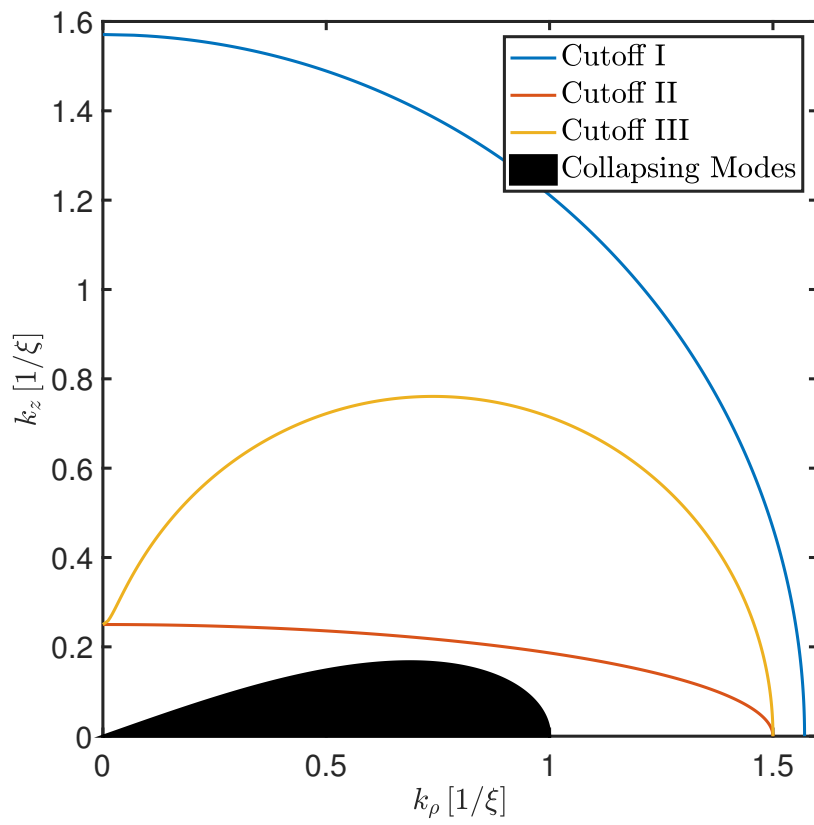


Figure 5.1: k -space cutoffs used in this work, and in the literature (see text).

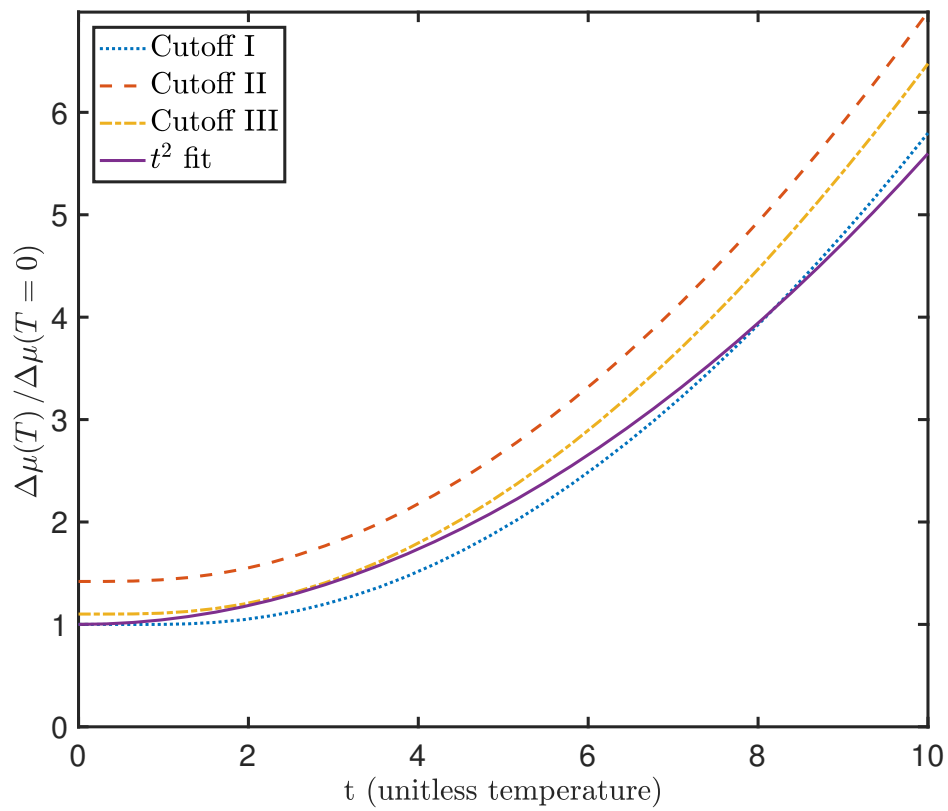


Figure 5.2: Temperature dependence of the correction term for different cutoff options for $\epsilon_{dd} = 1.43$.

Basic algebraic manipulations yield the Bogoliubov amplitudes:

$$\begin{aligned}
|u(\mathbf{x}, \mathbf{k})|^2 &= \frac{\varepsilon_{\mathbf{k}} + n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{2E(\mathbf{x}, \mathbf{k})} + \frac{1}{2} \\
|v(\mathbf{x}, \mathbf{k})|^2 &= \frac{\varepsilon_{\mathbf{k}} + n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{2E(\mathbf{x}, \mathbf{k})} - \frac{1}{2} \\
u(\mathbf{x}, \mathbf{k})v^*(\mathbf{x}, \mathbf{k}) &= \frac{n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{2E(\mathbf{x}, \mathbf{k})}.
\end{aligned} \tag{5.10}$$

Therefore, the correction terms become:

$$\Omega_n(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) \left\{ \frac{\varepsilon_{\mathbf{k}} + n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k}) - E(\mathbf{x}, \mathbf{k})}{2E(\mathbf{x}, \mathbf{k})} + N_B(E(\mathbf{x}, \mathbf{k})) \frac{\varepsilon_{\mathbf{k}} + n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{E(\mathbf{x}, \mathbf{k})} \right\} \tag{5.11}$$

$$\Omega_m(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) \left\{ -\frac{n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{2E(\mathbf{x}, \mathbf{k})} + \frac{n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{2\varepsilon_{\mathbf{k}}} - N_B(E(\mathbf{x}, \mathbf{k})) \frac{n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{E(\mathbf{x}, \mathbf{k})} \right\}, \tag{5.12}$$

where $\Omega_m(\mathbf{x})$ is properly renormalized by the second term in the brackets. Hence the total correction,

$$\begin{aligned}
\Delta\mu(\mathbf{x}) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}_{\text{int}}(\mathbf{k}) \left\{ \frac{\varepsilon_{\mathbf{k}}}{2E(\mathbf{x}, \mathbf{k})} + \frac{n_0(\mathbf{x})\tilde{V}_{\text{int}}(\mathbf{k})}{2\varepsilon_{\mathbf{k}}} - \frac{1}{2} \right. \\
&\quad \left. + \frac{1}{\exp[E(\mathbf{x}, \mathbf{k})/k_B T] - 1} \frac{\varepsilon_{\mathbf{k}}}{E(\mathbf{x}, \mathbf{k})} \right\}.
\end{aligned} \tag{5.13}$$

Using

$$\xi(\mathbf{x}) = \sqrt{\frac{\hbar^2}{2Mgn_0(\mathbf{x})}}, \tag{5.14}$$

$k = q/\xi$, $\cos\vartheta = u$, $f(u) = 1 + \varepsilon_{dd}(3u^2 - 1)$, and $t(\mathbf{x}) = \frac{k_B T}{gn_0(\mathbf{x})}$, one can write

$$\begin{aligned}
\Delta\mu(\mathbf{x}) &= \frac{g}{4\pi^2\xi^3(\mathbf{x})} \int_{-1}^1 du \int_{q_c}^{\infty} q^2 dq f(u) \left\{ \frac{q^2}{2\sqrt{q^2(q^2 + 2f(u))}} + \frac{f(u)}{2q^2} - \frac{1}{2} \right. \\
&\quad \left. + \frac{1}{\exp\left[\sqrt{q^2(q^2 + 2f(u))}/t(\mathbf{x})\right] - 1} \frac{q^2}{\sqrt{q^2(q^2 + 2f(u))}} \right\}
\end{aligned} \tag{5.15}$$

Since $\xi \propto \Psi^{-1}$, the local change in the chemical potential is

$$\Delta\mu(\mathbf{x}) = \frac{32}{3}g\sqrt{\frac{a_s^3}{\pi}} (\mathcal{Q}_5(\varepsilon_{dd}) + \mathcal{R}(\varepsilon_{dd}, t(\mathbf{x}))) |\Psi(\mathbf{x})|^3. \tag{5.16}$$

dimensionless functions \mathcal{Q}_5 and \mathcal{R} are given by

$$\mathcal{Q}_5(\epsilon_{dd}; q_c) = \frac{1}{4\sqrt{2}} \int_0^1 du f(u) \left[(4f(u) - q_c^2) \sqrt{2f(u) + q_c^2} - 3f(u)q_c + q_c^3 \right] \quad (5.17)$$

$$\mathcal{R}(\epsilon_{dd}, t; q_c) = \frac{3}{4\sqrt{2}} \int_0^1 du \int_{q_c^2}^{\infty} dQ \frac{Qf(u)}{\sqrt{Q + 2f(u)}} \frac{1}{\exp[\sqrt{Q(Q + 2f(u))}/t] - 1}. \quad (5.18)$$

Within the same local density approximation, the non-condensate density is given by

$$\tilde{n}(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} (|v(\mathbf{x}, \mathbf{k})|^2 + N_B(E(\mathbf{x}, \mathbf{k})) [|u(\mathbf{x}, \mathbf{k})|^2 + |v(\mathbf{x}, \mathbf{k})|^2]). \quad (5.19)$$

Using the Bogoliubov amplitudes given in Eq. 5.10, one finds

$$\tilde{n}(\mathbf{x}) = \frac{8}{3} \sqrt{\frac{a_s^3}{\pi}} (\mathcal{Q}_3(\epsilon_{dd}) + \mathcal{P}(\epsilon_{dd}, t(\mathbf{x}))) |\Psi(\mathbf{x})|^3, \quad (5.20)$$

where

$$\mathcal{Q}_3(\epsilon_{dd}; q_c) = \frac{1}{\sqrt{2}} \int_0^1 du f(u) \left[(f(u) - q_c^2) \sqrt{2f(u) + q_c^2} + q_c^3 \right] \quad (5.21)$$

$$\mathcal{P}(\epsilon_{dd}, t; q_c) = \frac{3}{\sqrt{2}} \int_0^1 du \int_{q_c^2}^{\infty} dQ \frac{Q + f(u)}{\sqrt{Q + 2f(u)}} \frac{1}{\exp[\sqrt{Q(Q + 2f(u))}/t] - 1}. \quad (5.22)$$

The non-condensate density increases with increasing temperature due to thermal depletion. In Fig. 5.3, temperature dependence of the non-condensate density is plotted. It is important to note that, near the edge of the condensate the dimensionless temperature (t) increases as the condensate density decreases. Although the fraction of the non-condensate to the condensate density increases near the edge, total number of depleted atoms can remain small. Therefore, we neglect the non-condensate density and the correction term $\Phi_1(\mathbf{x})$. Keeping \tilde{n} is also incompatible with the normalization condition of the condensate wavefunction.

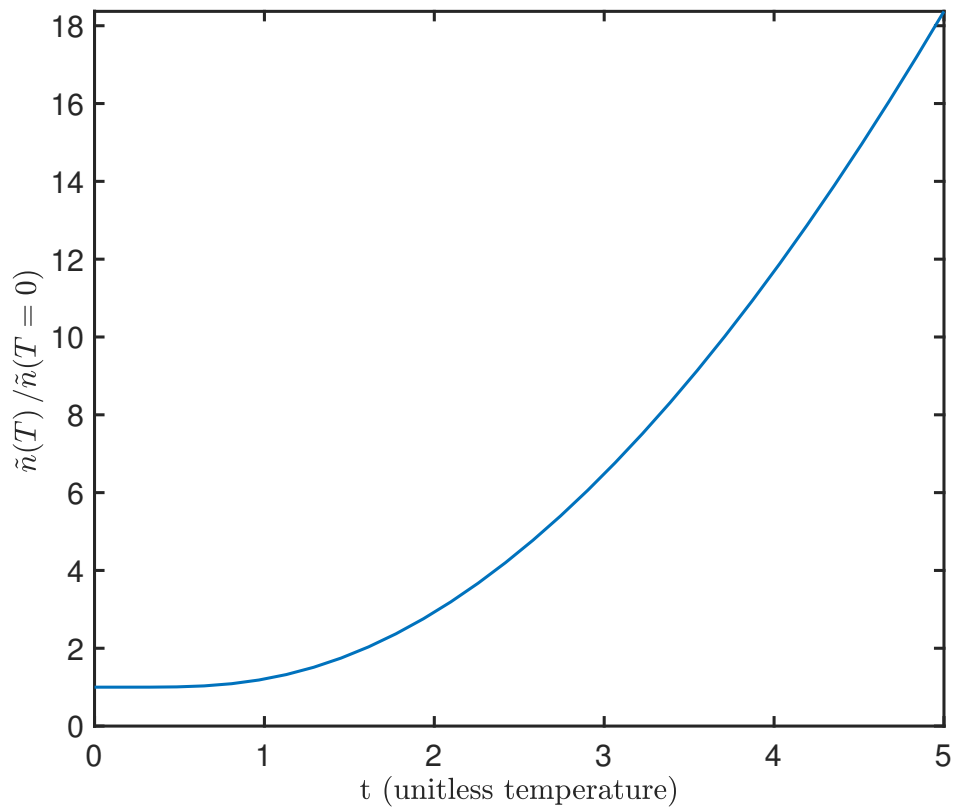


Figure 5.3: Non-condensate density as a function of dimensionless temperature.

Chapter 6

Variational Solution of the Modified Gross–Pitaevskii Equation

To estimate the temperature effects on the condensate, we employ a Gaussian variational ansatz. Energy functional corresponding to the modified Gross–Pitaevskii equation is similar to what is used in Ref. [16]. However, the thermal fluctuation term, \mathcal{R} , depends on condensate density through the dimensionless temperature. To get an analytical form for energy functional in Ψ , we used a power law fit for the \mathcal{R} function. A t^n curve for $n > 2.5$ results in a divergence near the condensate edge where the condensate density is low and the dimensionless temperature is high. This divergence is a byproduct of the Gaussian variational method, where the condensate extends to infinity. We find that a t^2 fit captures the trend of the \mathcal{R} function for numerically obtained values within $0 < t < 10$, and results in a finite correction when integrated over all space. In Fig. 5.2 of the text, we plot this fit with the function \mathcal{R}^1 .

Therefore, in the region where the depleted density is negligible compared to

¹The fit parameter in $\mathcal{R}(\epsilon_{dd}, t) = S(\epsilon_{dd})t^2$ is given by $S(\epsilon_{dd}) = -0.01029\epsilon_{dd}^4 + 0.02963\epsilon_{dd}^3 - 0.05422\epsilon_{dd}^2 + 0.009302\epsilon_{dd} + 0.1698$ for $0 < \epsilon_{dd} < 2$.

the condensate density, the modified Gross–Pitaevskii equation reads:

$$\left[\frac{\hbar^2}{2M} \nabla^2 + U_{\text{tr}}(\mathbf{x}) + \int d^3 \mathbf{x}' V_{\text{int}}(\mathbf{x} - \mathbf{x}') |\Psi(\mathbf{x}')|^2 + \gamma |\Psi(\mathbf{x})|^3 + \theta T^2 \frac{1}{|\Psi(\mathbf{x})|} \right] \Psi(\mathbf{x}) = \mu \Psi(\mathbf{x}), \quad (6.1)$$

where $\gamma = \frac{32}{3} g \sqrt{\frac{a_s^3}{\pi}} \mathcal{Q}_5(\epsilon_{dd})$, and $\theta = \frac{32}{3} g \sqrt{\frac{a_s^3}{\pi}} \frac{k_B^2}{g^2} \mathcal{S}(\epsilon_{dd})$, and \mathcal{S} is found from the t^2 fit.

We study dipolar Bose–Einstein condensates in two cases: static, and dynamic. In the static case, we use a time independent Gaussian variational ansatz, and minimize the energy functional corresponding to the modified Gross–Pitaevskii equation:

$$\begin{aligned} E[\Psi] = & \int d^3 \mathbf{x} \Psi^*(\mathbf{x}) \left[-\frac{\hbar^2}{2M} \nabla^2 + U_{\text{tr}}(\mathbf{x}) \right] \Psi(\mathbf{x}) \\ & + \frac{1}{2} \int d^3 \mathbf{x} \int d^3 \mathbf{x}' |\Psi(\mathbf{x})|^2 V_{\text{int}}(\mathbf{x} - \mathbf{x}') |\Psi(\mathbf{x}')|^2 \\ & + \frac{2}{5} \int d^3 \mathbf{x} \gamma |\Psi(\mathbf{x})|^5 \\ & + 2 \int d^3 \mathbf{x} \theta T^2 |\Psi(\mathbf{x})|. \end{aligned} \quad (6.2)$$

In the dynamic case, we utilize the Lagrangian of the system [15] with a time dependent Gaussian variational ansatz. We derive the Euler–Lagrange equations for the widths, and investigate the collective oscillations of the condensate. Since the time dependent case is more general, it suffices to work only with the Lagrangian as it includes the time independent solution.

Lagrangian density corresponding to the finite temperature equation in 6.1,

$$\begin{aligned} \mathcal{L} = & \frac{i\hbar}{2} \left(\Psi(\mathbf{x}, t) \frac{\partial \Psi^*(\mathbf{x}, t)}{\partial t} - \Psi^*(\mathbf{x}, t) \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} \right) + \frac{\hbar^2}{2M} |\nabla \Psi(\mathbf{x}, t)|^2 \\ & + U_{\text{tr}}(\mathbf{x}) |\Psi(\mathbf{x}, t)|^2 \\ & + \frac{1}{2} \int d^3 \mathbf{x}' |\Psi(\mathbf{x}, t)|^2 V_{\text{int}}(\mathbf{x} - \mathbf{x}') |\Psi(\mathbf{x}', t)|^2 \\ & + \frac{2}{5} \gamma |\Psi(\mathbf{x}, t)|^5 \\ & + 2\theta T^2 |\Psi(\mathbf{x}, t)|. \end{aligned} \quad (6.3)$$

The time dependent Gaussian anzats is

$$\begin{aligned} \Psi(x, y, z, t) = & \frac{\sqrt{N}}{\pi^{3/4} (w_x(t)w_y(t)w_z(t))^{1/2}} \\ & \times \exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x(t)^2} + \frac{y^2}{w_y(t)^2} + \frac{z^2}{w_z(t)^2} \right) \right. \\ & \left. + i (x^2 \beta_x(t) + y^2 \beta_y(t) + z^2 \beta_z(t)) \right], \end{aligned} \quad (6.4)$$

where w_i (width of the Gaussian wavefunction)² and β_i are the variational parameters.

The total Lagrangian, $L = \int d^3\mathbf{x} \mathcal{L}$, is obtained by inserting the Gaussian anzats given by Eq. 6.4 into the Lagrangian density equation. The Lagrangian reads (see: Appendix B):

$$\begin{aligned} L(w_x, w_y, w_z, \beta_x, \beta_y, \beta_z) = & \frac{N\hbar}{2} \left(w_x^2 \dot{\beta}_x + w_y^2 \dot{\beta}_y + w_z^2 \dot{\beta}_z \right) \\ & + \frac{\hbar^2 N}{4M} \left(\frac{1}{w_x^2} + \frac{1}{w_y^2} + \frac{1}{w_z^2} + 4w_x^2 \beta_x^2 + 4w_y^2 \beta_y^2 + 4w_z^2 \beta_z^2 \right) \\ & + \frac{1}{4} MN (\omega_x^2 w_x^2 + \omega_y^2 w_y^2 + \omega_z^2 w_z^2) \\ & + \frac{gN^2}{2} \frac{1}{2^{3/2} \pi^{3/2} w_x w_y w_z} \left(1 - \epsilon_{dd} F \left(\frac{w_x}{w_z}, \frac{w_y}{w_z} \right) \right) \\ & + \frac{4\sqrt{2}}{25\sqrt{5}\pi^{9/4}} \frac{N^{5/2} \gamma}{(w_x w_y w_z)^{3/2}} \\ & + 4\sqrt{2}\pi^{3/4} \theta T^2 N^{1/2} (w_x w_y w_z)^{1/2}, \end{aligned} \quad (6.5)$$

where $F(\kappa_x, \kappa_y)$ is the anistropy function calculated in Appendix B. We write the Lagrangian per particle as,

$$\frac{1}{N} L = \frac{\hbar}{2} \left(w_x^2 \dot{\beta}_x + w_y^2 \dot{\beta}_y + w_z^2 \dot{\beta}_z \right) + \frac{\hbar^2}{M} \left(w_x^2 \beta_x^2 + w_y^2 \beta_y^2 + w_z^2 \beta_z^2 \right) + G(w_x, w_y, w_z), \quad (6.6)$$

²In figures $\sigma_i = 2w_i$ are used.

where

$$\begin{aligned}
G(w_x, w_y, w_z) = & \frac{\hbar^2}{4M} \left(\frac{1}{w_x^2} + \frac{1}{w_y^2} + \frac{1}{w_z^2} \right) + \frac{1}{4}M (\omega_x^2 w_x^2 + \omega_y^2 w_y^2 + \omega_z^2 w_z^2) \\
& + \frac{gN}{2} \frac{1}{2^{3/2} \pi^{3/2} w_x w_y w_z} \left(1 - \epsilon_{dd} F \left(\frac{w_x}{w_z}, \frac{w_y}{w_z} \right) \right) \\
& + \frac{4\sqrt{2}}{25\sqrt{5}\pi^{9/4}} \frac{N^{3/2}\gamma}{(w_x w_y w_z)^{3/2}} + 4\sqrt{2}\pi^{3/4}\theta T^2 N^{-1/2} (w_x w_y w_z)^{1/2}
\end{aligned} \tag{6.7}$$

Solving the Euler–Lagrange equations for the parameters w_η and β_η , we find the equation of motion for the width of the condensate.

$$\frac{d^2 w_\eta}{dt^2} = -\frac{2}{M} \frac{\partial}{\partial w_\eta} G(w_x, w_y, w_z). \tag{6.8}$$

First, we find the equilibrium via

$$\left. \frac{\partial G}{\partial w_\eta} \right|_{w_{\eta(0)}} = 0. \tag{6.9}$$

Then, we expand $G(w_x, w_y, w_z)$ around the minimum,

$$\begin{aligned}
G(w_{x(0)} + \delta_x, w_{y(0)} + \delta_y, w_{z(0)} + \delta_z) = & G(w_{x(0)}, w_{y(0)}, w_{z(0)}) \\
& + \frac{1}{2} \delta_x^2 \left. \frac{\partial^2 G}{\partial w_x^2} \right|_{(0)} + \frac{1}{2} \delta_y^2 \left. \frac{\partial^2 G}{\partial w_y^2} \right|_{(0)} + \frac{1}{2} \delta_z^2 \left. \frac{\partial^2 G}{\partial w_z^2} \right|_{(0)} \\
& + \delta_x \delta_y \left. \frac{\partial^2 G}{\partial w_x \partial w_y} \right|_{(0)} + \delta_y \delta_z \left. \frac{\partial^2 G}{\partial w_y \partial w_z} \right|_{(0)} \\
& + \delta_z \delta_x \left. \frac{\partial^2 G}{\partial w_z \partial w_x} \right|_{(0)}.
\end{aligned} \tag{6.10}$$

Defining $k_\eta = \left. \frac{\partial^2 G}{\partial w_\eta^2} \right|_{(0)}$, $\lambda_{\alpha,\beta} = \left. \frac{\partial^2 G}{\partial w_\alpha \partial w_\beta} \right|_{(0)}$, and the matrix

$$M = \frac{2}{M} \begin{bmatrix} k_x & \lambda_{xy} & \lambda_{zx} \\ \lambda_{xy} & k_y & \lambda_{yz} \\ \lambda_{zx} & \lambda_{yz} & k_z \end{bmatrix}, \tag{6.11}$$

we reduce the problem to diagonalizing the matrix above (called Hessian). The eigenvalues of this matrix are the three oscillation frequencies(-squared) for the condensate widths. The eigenvectors indicate the principal directions for these

oscillations, thus the nature of the collective oscillation modes. In a cylindrically symmetric trap, one eigenvector is always $[1/\sqrt{2}, -1/\sqrt{2}, 0]$. This is called the $x - y$ mode. The other two are monopole and quadrupole oscillations. The eigenvectors corresponding to these two modes are of the forms $[1, 1, -v]$ and $[1, 1, +v]$, respectively. Pictorially, quadrupole mode, also called axial mode, is when height (width in z direction) changes opposite to radius (width in ρ direction). Monopole mode, also called breathing mode, is when all three widths change in phase.

Chapter 7

Results and Conclusion

We study the two systems reported in [8] and [13] in both static and dynamic cases. In the static case, we focus on the widths of these droplets. In the dynamic case, using the Lagrangian machinery, we calculate the oscillation frequencies of condensate widths.

The first system that we investigate is similar to what is reported in [8], where 2000 ^{164}Dy atoms are confined by the trapping potential $\{\omega_\rho, \omega_z\} = \{45, 133\} \text{ s}^{-1}$. Dipolar length is $a_{dd} = 132 a_0$, and the s-wave scattering length is $a_s = 93 a_0$, where $a_0 = 5.29 \times 10^{-11} \text{ m}$ is the Bohr radius.

This system favors lower density phase at zero temperature, but as temperature increases cigar shaped high density (droplet) phase become energetically favorable Fig. 7.1. In most other conditions, this behavior is absent because the condensate strongly favors one of the two phases. However, near bi-stability, where at zero temperature two solutions both exist, condensate shape may be temperature dependent. This transition to droplet phase occurs near 100nK which is relevant in the experimental setups that these droplets are observed.

The second system we studied is the Innsbruck group's macro-droplet, where 20000 ^{166}Er atoms are held in a prolate trap $\{\omega_\rho, \omega_z\} = \{178, 17.2\} \text{ s}^{-1}$. Dipolar length of the erbium atoms is $a_{dd} = 65.5 a_0$, and the s-wave scattering length

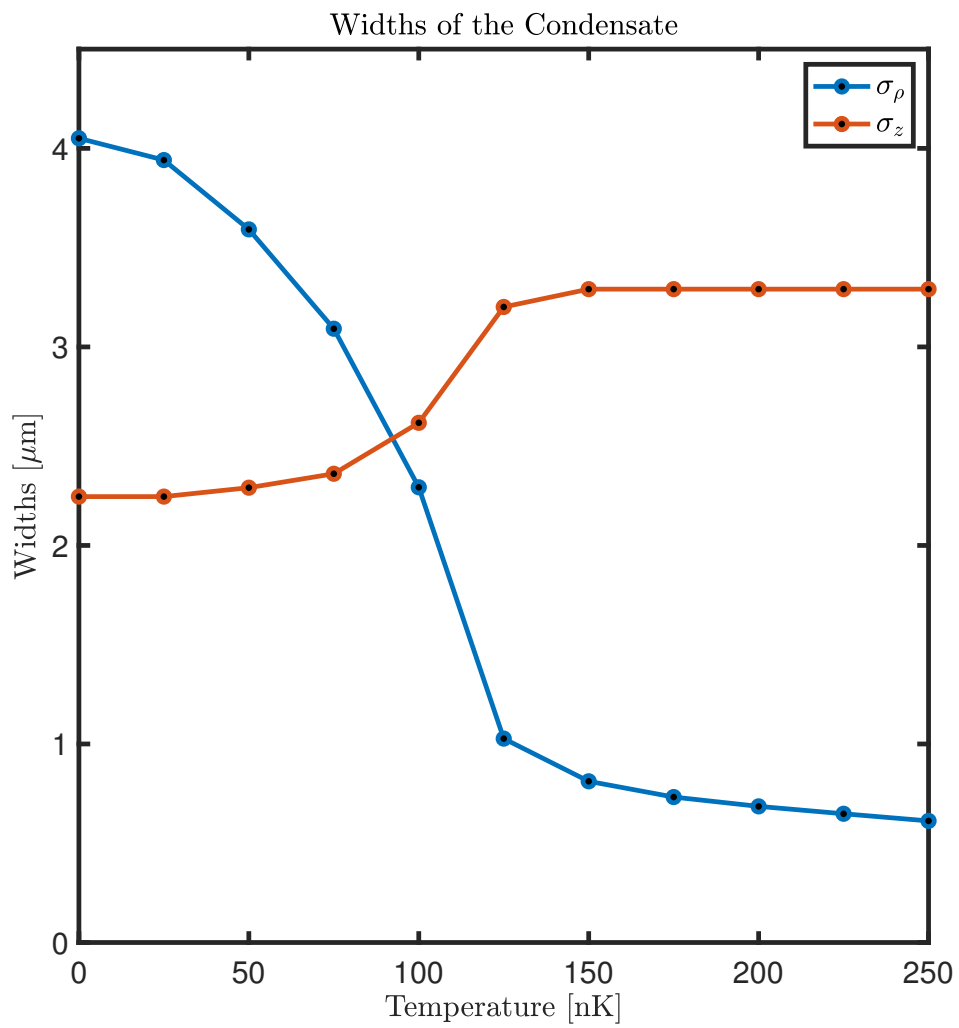


Figure 7.1: Droplet widths in dysprosium experiment.

is near $a_s = 60 a_0$ in the reported droplet experiment [13]. The only phase supported in this trap is the droplet phase. Still, as temperature increases to 300nK, the condensate shrinks in size in about 20% (Fig. 7.2). As absolute control of temperature is not possible in experiments, this change in size may be lost in the imaging resolution in the experiments.

Collective oscillations of these two systems also show the temperature dependency. The dysprosium droplet's collective oscillation frequencies are highly temperature dependent Fig. 7.3. However, since this condensate is fairly small, and hard to image, the collective oscillations may not be observed as easily as the condensate shape.

In the case of a large droplet, monitoring the collective oscillation of the droplet along its long axis is possible [13]. Fig. 7.4 shows that the axial mode frequency increases by about 40% in a temperature range 0 – 300nK.

This study on the shape and the collective oscillations of the dipolar droplets can be made more rigorous in a couple of ways. First, the correction term may be calculated with a better approximation which will not need an arbitrary choice of cut off. Second, the fourth order terms in the Hamiltonian can be incorporated into the Bogoliubov–de Gennes equations making them self-consistent, albeit non-linear. Third, a numerical solver can be implemented to self-consistently solve the modified Gross–Pitaevskii equation and the modified Bogoliubov–de Gennes equations. Furthermore, since the beyond mean field effects are prevalent, a non-perturbative picture may be needed to fully understand the system.

We conclude that temperature fluctuations are important in determining the condensate shape and the collective oscillations. In the future, a more precise investigation may provide a means to probe temperature in Bose–Einstein condensates.

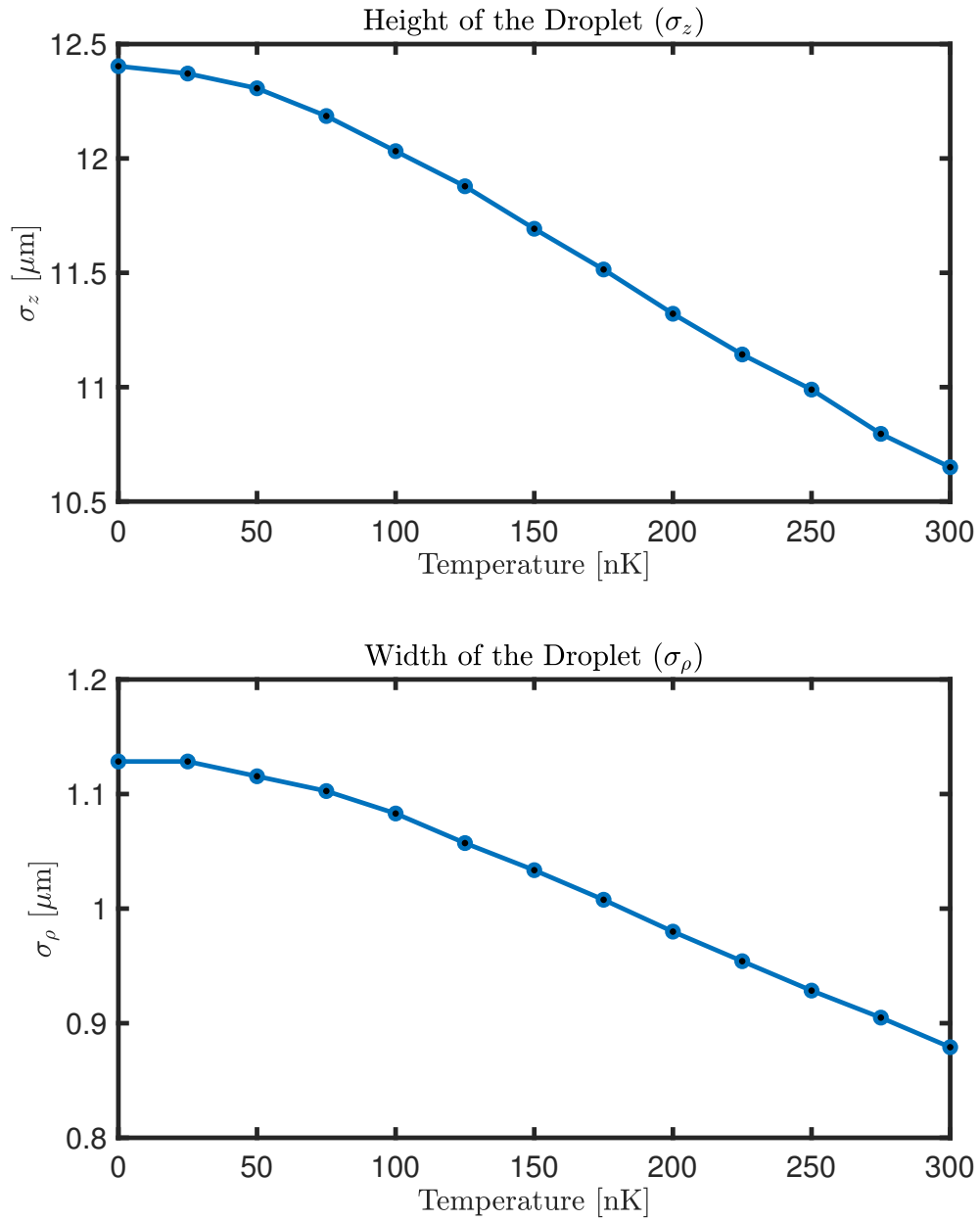


Figure 7.2: Droplet widths in erbium experiment.

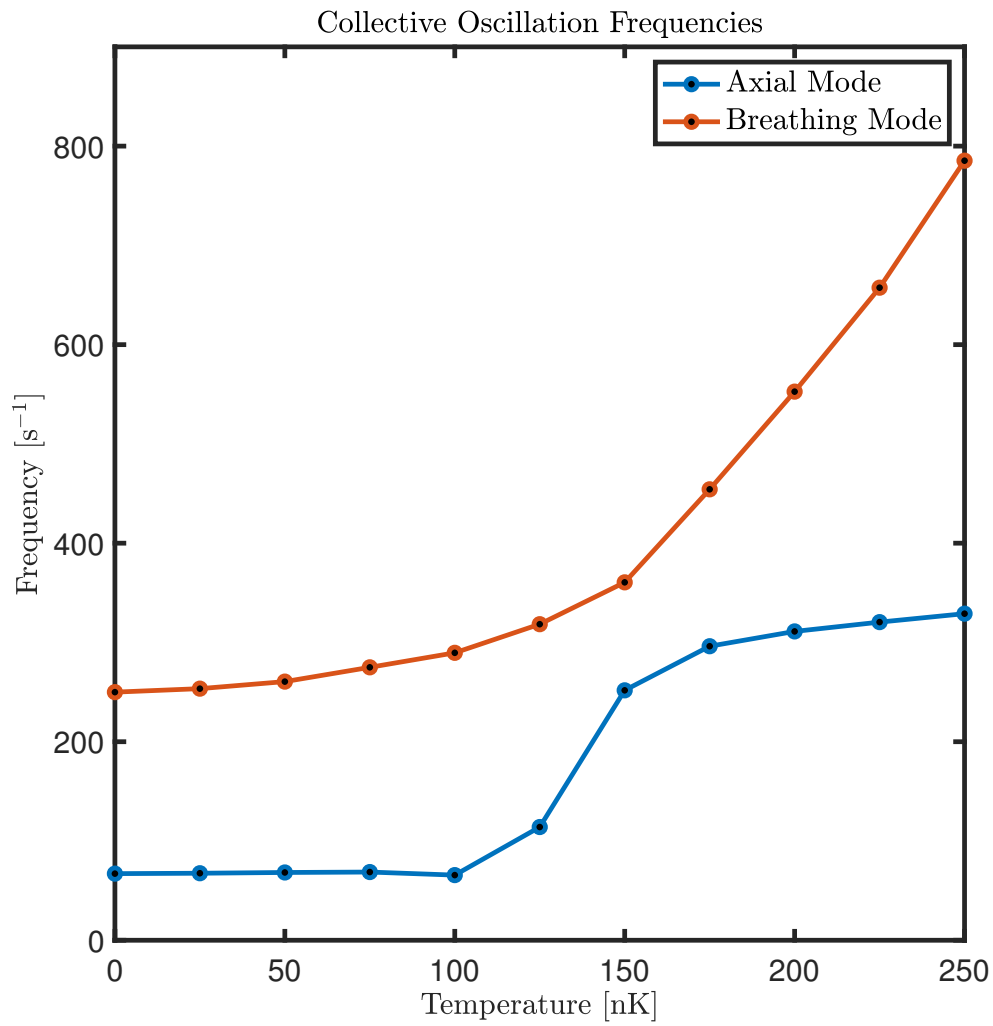


Figure 7.3: Temperature dependence of the two collective oscillations in dysprosium experiment.

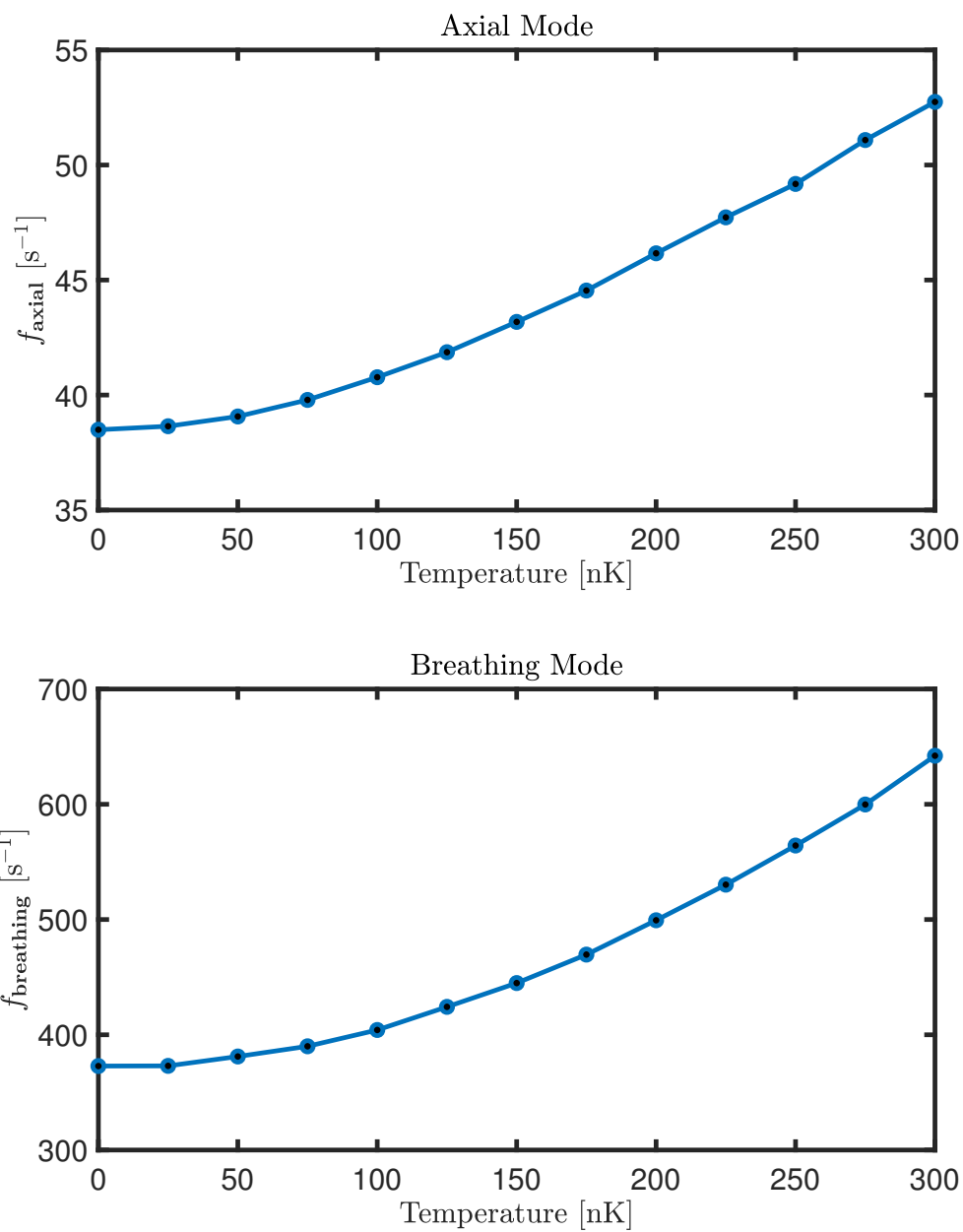


Figure 7.4: Temperature dependence of the two collective oscillations in erbium experiment.

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Appendix A

Derivation of the Bogoliubov–de Gennes Equations

With the Bogoliubov transformation, the \hat{H}_2 becomes:

$$\begin{aligned}
\hat{H}_2 = & \sum_{j,k} \int d^3\mathbf{x} \left(u_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger - v_j(\mathbf{x}) \hat{\alpha}_j \right) \left(-\frac{\hbar^2 \nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) \left(u_k(\mathbf{x}) \hat{\alpha}_k - v_k^*(\mathbf{x}) \hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \left(u_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger - v_j(\mathbf{x}) \hat{\alpha}_j \right) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \left(u_k(\mathbf{x}) \hat{\alpha}_k - v_k^*(\mathbf{x}) \hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \left(u_j^*(\mathbf{x}') \hat{\alpha}_j^\dagger - v_j(\mathbf{x}') \hat{\alpha}_j \right) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \left(u_k(\mathbf{x}') \hat{\alpha}_k - v_k^*(\mathbf{x}') \hat{\alpha}_k^\dagger \right) \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \left(u_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger - v_j(\mathbf{x}) \hat{\alpha}_j \right) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \left(u_k(\mathbf{x}') \hat{\alpha}_k - v_k^*(\mathbf{x}') \hat{\alpha}_k^\dagger \right) \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \left(u_j^*(\mathbf{x}') \hat{\alpha}_j^\dagger - v_j(\mathbf{x}') \hat{\alpha}_j \right) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \left(u_k(\mathbf{x}) \hat{\alpha}_k - v_k^*(\mathbf{x}) \hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \left(u_j(\mathbf{x}') \hat{\alpha}_j - v_j^*(\mathbf{x}') \hat{\alpha}_j^\dagger \right) \left(u_k(\mathbf{x}) \hat{\alpha}_k - v_k^*(\mathbf{x}) \hat{\alpha}_k^\dagger \right) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \left(u_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger - v_j(\mathbf{x}) \hat{\alpha}_j \right) \left(u_k^*(\mathbf{x}') \hat{\alpha}_k^\dagger - v_k(\mathbf{x}') \hat{\alpha}_k \right) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}).
\end{aligned} \tag{A.1}$$

To diagonalize the Hamiltonian above, we dissect it in terms of the quasi particle operator combinations:

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j^\dagger\hat{\alpha}_k\} = & \sum_{j,k} \left(\int d^3\mathbf{x} u_j^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) u_k(\mathbf{x}) \right. \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_k(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) u_j^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') u_k(\mathbf{x}') \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') u_k(\mathbf{x}') \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) u_j^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_k(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') v_j^*(\mathbf{x}') u_k(\mathbf{x}) \\
& \left. - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) v_k(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}) \right) \times \left(\hat{\alpha}_j^\dagger \hat{\alpha}_k \right), \tag{A.2}
\end{aligned}$$

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j\hat{\alpha}_k^\dagger\} = & \sum_{j,k} \left(\int d^3\mathbf{x} v_j(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) v_k^*(\mathbf{x}) \right. \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_k^*(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) v_j(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') v_k^*(\mathbf{x}') \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') v_k^*(\mathbf{x}') \Psi(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) v_j(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_k^*(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') u_j(\mathbf{x}') v_k^*(\mathbf{x}) \\
& \left. - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) u_k^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}) \right) \times \left(\hat{\alpha}_j \hat{\alpha}_k^\dagger \right), \tag{A.3}
\end{aligned}$$

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j\hat{\alpha}_k\} = & \sum_{j,k} \left(- \int d^3\mathbf{x} v_j(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) u_k(\mathbf{x}) \right. \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_k(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) v_j(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') u_k(\mathbf{x}') \Psi(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') u_k(\mathbf{x}') \Psi(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) v_j(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_k(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') u_j(\mathbf{x}') u_k(\mathbf{x}) \\
& \left. + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) v_k(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}) \right) \times (\hat{\alpha}_j \hat{\alpha}_k),
\end{aligned} \tag{A.4}$$

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j^\dagger \hat{\alpha}_k^\dagger\} = & \sum_{j,k} \left(- \int d^3\mathbf{x} u_j^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) \right) v_k^*(\mathbf{x}) \right. \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_k^*(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) u_j^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') v_k^*(\mathbf{x}') \Psi(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') v_k^*(\mathbf{x}') \Psi(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) u_j^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_k^*(\mathbf{x}) \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' \Psi^*(\mathbf{x}) \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') v_j^*(\mathbf{x}') v_k^*(\mathbf{x}) \\
& \left. + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) u_k^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}) \right) \times (\hat{\alpha}_j^\dagger \hat{\alpha}_k^\dagger).
\end{aligned} \tag{A.5}$$

Using $\int d^3\mathbf{x} f(\mathbf{x}) \nabla^2 g(\mathbf{x}) = \int d^3\mathbf{x} g(\mathbf{x}) \nabla^2 f(\mathbf{x})$ for square integrable functions f and g , and introducing the Hartree potential

$$\Phi_0(\mathbf{x}) = \int d^3\mathbf{x}' \Psi^*(\mathbf{x}') V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}'), \tag{A.6}$$

we rewrite the terms above in a symmetrical manner

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j^\dagger\hat{\alpha}_k\} &= \sum_{j,k} \left(\frac{1}{2} \int d^3\mathbf{x} u_j^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u_k(\mathbf{x}) \right. \\
&\quad + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') u_k(\mathbf{x}') \\
&\quad - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_k(\mathbf{x}') \\
&\quad + \frac{1}{2} \int d^3\mathbf{x} u_k(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u_j^*(\mathbf{x}) \\
&\quad + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_k(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_j^*(\mathbf{x}') \\
&\quad \left. - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_k(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') v_j^*(\mathbf{x}') \right) \times \left(\hat{\alpha}_j^\dagger \hat{\alpha}_k \right), \tag{A.7}
\end{aligned}$$

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j\hat{\alpha}_k^\dagger\} &= \sum_{j,k} \left(\frac{1}{2} \int d^3\mathbf{x} v_j(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) v_k^*(\mathbf{x}) \right. \\
&\quad + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') v_k^*(\mathbf{x}') \\
&\quad - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_k^*(\mathbf{x}') \\
&\quad + \frac{1}{2} \int d^3\mathbf{x} v_k^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) v_j(\mathbf{x}) \\
&\quad + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_k^*(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_j(\mathbf{x}') \\
&\quad \left. - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_k^*(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') u_j(\mathbf{x}') \right) \times \left(\hat{\alpha}_j \hat{\alpha}_k^\dagger \right), \tag{A.8}
\end{aligned}$$

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j\hat{\alpha}_k\} = & \sum_{j,k} \left(-\frac{1}{2} \int d^3\mathbf{x} v_j(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u_k(\mathbf{x}) \right. \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') u_k(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_j(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_k(\mathbf{x}') \\
& - \frac{1}{2} \int d^3\mathbf{x} u_k(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) v_j(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_k(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_j(\mathbf{x}') \\
& \left. + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_k(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') u_j(\mathbf{x}') \right) \times (\hat{\alpha}_j\hat{\alpha}_k), \tag{A.9}
\end{aligned}$$

$$\begin{aligned}
\hat{H}_2\{\hat{\alpha}_j^\dagger\hat{\alpha}_k^\dagger\} = & \sum_{j,k} \left(-\frac{1}{2} \int d^3\mathbf{x} u_j^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) v_k^*(\mathbf{x}) \right. \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') v_k^*(\mathbf{x}') \\
& + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' u_j^*(\mathbf{x}) \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_k^*(\mathbf{x}') \\
& - \frac{1}{2} \int d^3\mathbf{x} v_k^*(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u_j^*(\mathbf{x}) \\
& - \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_k^*(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') u_j^*(\mathbf{x}') \\
& \left. + \frac{1}{2} \iint d^3\mathbf{x} d^3\mathbf{x}' v_k^*(\mathbf{x}) \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') v_j^*(\mathbf{x}') \right) \times (\hat{\alpha}_j^\dagger\hat{\alpha}_k^\dagger). \tag{A.10}
\end{aligned}$$

It is now apparent that, if u and v obey the coupled equations, called Bogoliubov–de Gennes equations:

$$\begin{aligned}
\left(-\frac{\hbar^2\nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) u_j(\mathbf{x}) + \int d^3\mathbf{x}' \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') u_j(\mathbf{x}') \\
- \int d^3\mathbf{x}' \Psi(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_j(\mathbf{x}') = E_j u_j(\mathbf{x}), \tag{A.11}
\end{aligned}$$

$$\begin{aligned}
& \left(-\frac{\hbar^2 \nabla^2}{2M} - \mu + U_{\text{tr}}(\mathbf{x}) + \Phi_0(\mathbf{x}) \right) v_j(\mathbf{x}) + \int d^3 \mathbf{x}' \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') v_j(\mathbf{x}') \\
& - \int d^3 \mathbf{x}' \Psi^*(\mathbf{x}) V_{\text{int}}(\mathbf{x} - \mathbf{x}') \Psi^*(\mathbf{x}') u_j(\mathbf{x}') = -E_j v_j(\mathbf{x}),
\end{aligned} \tag{A.12}$$

the Hamiltonian is diagonalized (see Chapter 4).

Appendix B

Calculation of the Lagrangian with the Gaussian Ansatz

B.1 The Lagrangian of the Gaussian Ansatz

We start with the time dependent Gaussian ansatz:

$$\begin{aligned} \Psi(x, y, z, t) = & \frac{\sqrt{N}}{\pi^{3/4} (w_x(t)w_y(t)w_z(t))^{1/2}} \\ & \times \exp\left[-\frac{1}{2} \left(\frac{x^2}{w_x(t)^2} + \frac{y^2}{w_y(t)^2} + \frac{z^2}{w_z(t)^2} \right) \right. \\ & \left. + i (x^2\beta_x(t) + y^2\beta_y(t) + z^2\beta_z(t))\right], \end{aligned} \quad (\text{B.1})$$

where w_i (width of the Gaussian wavefunction) and β_i are the variational parameters. Lagrangian density is,

$$\begin{aligned}\mathcal{L} = & \frac{i\hbar}{2} \left(\Psi(\mathbf{x}, t) \frac{\partial \Psi^*(\mathbf{x}, t)}{\partial t} - \Psi^*(\mathbf{x}, t) \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} \right) + \frac{\hbar^2}{2M} |\nabla \Psi(\mathbf{x}, t)|^2 \\ & + U_{\text{tr}}(\mathbf{x}) |\Psi(\mathbf{x}, t)|^2 \\ & + \frac{1}{2} \int d^3 \mathbf{x}' |\Psi(\mathbf{x}, t)|^2 V_{\text{int}}(\mathbf{x} - \mathbf{x}') |\Psi(\mathbf{x}', t)|^2 \\ & + \frac{2}{5} \gamma |\Psi(\mathbf{x}, t)|^5 \\ & + 2\theta T^2 |\Psi(\mathbf{x}, t)|.\end{aligned}$$

The Lagrangian, $L = \int d^3 \mathbf{x} \mathcal{L}$, is obtained inserting the Gaussian anzats into the Lagrangian density equation.

B.1.1 Terms of $|\Psi|^n$ form

$|\Psi|^n$ reads:

$$|\Psi(\mathbf{x}, t)|^n = \frac{N^{n/2}}{\pi^{3n/4} (w_x w_y w_z)^{n/2}} \exp \left[-\frac{n}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) \right]. \quad (\text{B.2})$$

Therefore,

$$\int d^3 \mathbf{x} |\Psi(\mathbf{x}, t)|^n = \frac{N^{n/2}}{\pi^{3n/4} (w_x w_y w_z)^{n/2}} \left(\frac{2\pi}{n} \right)^{3/2} w_x w_y w_z. \quad (\text{B.3})$$

Hence,

$$\int d^3 \mathbf{x} \frac{2}{5} \gamma |\Psi(\mathbf{x}, t)|^5 = \frac{4\sqrt{2}}{25\sqrt{5}\pi^{9/4}} \frac{N^{5/2} \gamma}{(w_x w_y w_z)^{3/2}}, \quad (\text{B.4})$$

and

$$\int d^3 \mathbf{x} 2\theta T^2 |\Psi(\mathbf{x}, t)| = 4\sqrt{2}\pi^{3/4} \theta T^2 N^{1/2} (w_x w_y w_z)^{1/2}. \quad (\text{B.5})$$

B.1.2 Trap energy term

With the trap potential given by $U_{\text{tr}}(\mathbf{x}) = \frac{1}{2}M (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$,

$$\int d^3\mathbf{x} U_{\text{tr}}(\mathbf{x}) |\Psi(\mathbf{x}, t)|^2 = \int d^3\mathbf{x} \frac{1}{2}M (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \frac{N}{\pi^{3/2} w_x w_y w_z} \times \exp \left[-\frac{x^2}{w_x^2} - \frac{y^2}{w_y^2} - \frac{z^2}{w_z^2} \right]. \quad (\text{B.6})$$

Therefore,

$$E_{\text{tr}} = \frac{1}{4}MN (\omega_x^2 w_x^2 + \omega_y^2 w_y^2 + \omega_z^2 w_z^2) \quad (\text{B.7})$$

B.1.3 Interaction term

In the calculation of the interaction term, the following integral will be useful:

$$I(\eta, \lambda) = \int d^3\mathbf{x} \exp [-(\eta x^2 + \eta^{-1} y^2 + \lambda^2 z^2)] \frac{z^2}{x^2 + y^2 + z^2}. \quad (\text{B.8})$$

Note,

$$I(\eta, \lambda) = -\frac{\partial}{\partial \lambda^2} \int d^3\mathbf{x} \frac{\exp [-(\eta x^2 + \eta^{-1} y^2 + \lambda^2 z^2)]}{x^2 + y^2 + z^2}. \quad (\text{B.9})$$

Defining,

$$\begin{aligned} J(\eta, \lambda) &= \int d^3\mathbf{x} \frac{\exp [-(\eta x^2 + \eta^{-1} y^2 + \lambda^2 z^2)]}{x^2 + y^2 + z^2} \\ &= \int_0^\infty r^2 dr \int_0^{2\pi} d\phi \int_{-1}^1 d \cos \theta \frac{\exp [-r^2 (\sin^2 \theta (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi) + \lambda^2 \cos^2 \theta)]}{r^2} \\ &= \int_0^{2\pi} d\phi \int_{-1}^1 d \cos \theta \int_0^\infty dr \exp [-r^2 (\sin^2 \theta (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi) + \lambda^2 \cos^2 \theta)] \\ &= \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \frac{\sqrt{\pi}}{2} \frac{1}{\sqrt{\sin^2 \theta (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi) + \lambda^2 \cos^2 \theta}} \\ &= \sqrt{\pi} \int_0^{2\pi} d\phi \frac{1}{\sqrt{\lambda^2 - (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi)}} \tanh^{-1} \left[\frac{\sqrt{\lambda^2 - (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi)}}{\lambda} \right]. \end{aligned}$$

Let $\mu = \sqrt{\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi}$, then

$$\frac{\partial}{\partial \lambda^2} \frac{\tanh^{-1} \left[\frac{\sqrt{\lambda^2 - \mu^2}}{\sqrt{\lambda^2}} \right]}{\sqrt{\lambda^2 - \mu^2}} = \frac{1}{2} \left(\frac{1}{\lambda(\lambda^2 - \mu^2)} - \frac{\tanh^{-1} \left[\frac{\sqrt{\lambda^2 - \mu^2}}{\sqrt{\lambda^2}} \right]}{(\lambda^2 - \mu^2)^{3/2}} \right). \quad (\text{B.10})$$

Hence,

$$I(\eta, \lambda) = \frac{\sqrt{\pi}}{2} \int_0^{2\pi} d\phi \left(\frac{\tanh^{-1} \left[\frac{\sqrt{\lambda^2 - (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi)}}{\sqrt{\lambda^2}} \right]}{(\lambda^2 - (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi))^{3/2}} - \frac{1}{\lambda(\lambda^2 - (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi))} \right). \quad (\text{B.11})$$

If $\kappa = 1/\lambda$,

$$I(\eta, 1/\kappa) = \frac{\sqrt{\pi}}{2} \int_0^{2\pi} d\phi \left(\frac{\kappa^3 \tanh^{-1} \left[\frac{\sqrt{1 - \kappa^2 (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi)}}{\sqrt{\lambda^2}} \right]}{(1 - \kappa^2 (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi))^{3/2}} - \frac{\kappa^3}{1 - \kappa^2 (\eta \cos^2 \phi + \eta^{-1} \sin^2 \phi)} \right). \quad (\text{B.12})$$

The interaction energy,

$$\begin{aligned} E_{\text{int}} &= \frac{1}{2} \int d^3 \mathbf{x} \int d^3 \mathbf{x}' |\Psi(\mathbf{x}, t)|^2 V_{\text{int}}(\mathbf{x} - \mathbf{x}') |\Psi(\mathbf{x}', t)|^2 \\ &= \frac{1}{2} \int d^3 \mathbf{x} \int d^3 \mathbf{x}' \frac{N^2}{\pi^3 w_x^2 w_y^2 w_z^2} \exp \left[-\frac{x^2}{w_x^2} - \frac{y^2}{w_y^2} - \frac{z^2}{w_z^2} \right] V_{\text{int}}(\mathbf{x} - \mathbf{x}') \exp \left[-\frac{x'^2}{w_x^2} - \frac{y'^2}{w_y^2} - \frac{z'^2}{w_z^2} \right] \\ &= \frac{1}{2} g N^2 \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \exp \left[-\frac{1}{2} (k_x^2 w_x^2 + k_y^2 w_y^2 + k_z^2 w_z^2) \right] \left(1 + \epsilon_{dd} \left(\frac{3k_z^2}{k_x^2 + k_y^2 + k_z^2} - 1 \right) \right). \end{aligned} \quad (\text{B.13})$$

Let $\mathbf{q} = \sqrt{\frac{w_x w_y}{2}} \mathbf{k}$, then

$$\begin{aligned} E_{\text{int}} &= \frac{1}{2} g N^2 \frac{2^{3/2}}{(w_x w_y)^{3/2}} \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \exp \left[- (q_x^2 (w_x/w_y) + q_y^2 (w_y/w_x) + q_z^2 (w_z^2/w_x w_y)) \right] \\ &\quad \times \left(1 + \epsilon_{dd} \left(\frac{3q_z^2}{q_x^2 + q_y^2 + q_z^2} - 1 \right) \right) \\ &= \frac{g N^2}{2} \frac{1}{2^{3/2} \pi^3 (w_x w_y)^{3/2}} \left((1 - \epsilon_{dd}) \pi^{3/2} \frac{\sqrt{w_x w_y}}{w_z} + 3\epsilon_{dd} I \left(\frac{w_x}{w_y}, \frac{\sqrt{w_x w_y}}{w_z} \right) \right) \\ &= \frac{g N^2}{2} \frac{1}{2^{3/2} \pi^{3/2} w_x w_y w_z} \left(1 - \epsilon_{dd} F \left(\frac{w_x}{w_z}, \frac{w_y}{w_z} \right) \right), \end{aligned} \quad (\text{B.14})$$

where

$$F(\kappa_x, \kappa_y) = 1 - 3\kappa_x\kappa_y \int_0^\pi \frac{d\phi}{\pi} \left(\frac{\tanh^{-1} \left[\sqrt{1 - (\kappa_x^2 \cos^2 \phi + \kappa_y^2 \sin^2 \phi)} \right]}{(1 - (\kappa_x^2 \cos^2 \phi + \kappa_y^2 \sin^2 \phi))^{3/2}} - \frac{1}{1 - (\kappa_x^2 \cos^2 \phi + \kappa_y^2 \sin^2 \phi)} \right). \quad (\text{B.15})$$

B.1.4 Time derivatives

For the first term in the Lagrangian density, one needs to evaluate:

$$\frac{\partial \Psi(x, y, z, t)}{\partial t} = \frac{\partial}{\partial t} \left(\frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right] \right) \quad (\text{B.16})$$

$$\begin{aligned} \frac{\partial \Psi(x, y, z, t)}{\partial t} &= \frac{\partial}{\partial t} \left(\frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \right) \exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right] \\ &\quad + \frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \frac{\partial}{\partial t} \left(\exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right] \right) \\ &= \frac{\partial}{\partial t} \left(\frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \right) \exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right] \\ &\quad + \frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \frac{\partial}{\partial t} \left(-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right) \exp[\dots]. \end{aligned}$$

Hence,

$$\begin{aligned} \Psi^* \frac{\partial \Psi}{\partial t} &= \frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \frac{\partial}{\partial t} \left(\frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \right) \exp \left[-\frac{x^2}{w_x^2} - \frac{y^2}{w_y^2} - \frac{z^2}{w_z^2} \right] \\ &\quad + \frac{N}{\pi^{3/2} w_x w_y w_z} \frac{\partial}{\partial t} \left(-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right) \\ &\quad \times \exp \left[-\frac{x^2}{w_x^2} - \frac{y^2}{w_y^2} - \frac{z^2}{w_z^2} \right]. \quad (\text{B.17}) \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{i\hbar}{2} \left(\Psi(\mathbf{x}, t) \frac{\partial \Psi^*(\mathbf{x}, t)}{\partial t} - \Psi^*(\mathbf{x}, t) \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} \right) &= \\ \frac{N\hbar}{\pi^{3/2} w_x w_y w_z} \left(x^2 \dot{\beta}_x + y^2 \dot{\beta}_y + z^2 \dot{\beta}_z \right) \exp \left[-\frac{x^2}{w_x^2} - \frac{y^2}{w_y^2} - \frac{z^2}{w_z^2} \right]. \quad (\text{B.18}) \end{aligned}$$

Finally, integrating over the space yields,

$$\int d^3\mathbf{x} \frac{i\hbar}{2} \left(\Psi(\mathbf{x}, t) \frac{\partial \Psi^*(\mathbf{x}, t)}{\partial t} - \Psi^*(\mathbf{x}, t) \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} \right) = \frac{N\hbar}{2} \left(w_x^2 \dot{\beta}_x + w_y^2 \dot{\beta}_y + w_z^2 \dot{\beta}_z \right). \quad (\text{B.19})$$

B.1.5 $|\nabla\Psi|^2$ term

$$|\nabla\Psi(\mathbf{x}, t)|^2 = \left| \frac{\partial \Psi(x, y, z, t)}{\partial x} \right|^2 + \left| \frac{\partial \Psi(x, y, z, t)}{\partial y} \right|^2 + \left| \frac{\partial \Psi(x, y, z, t)}{\partial z} \right|^2 \quad (\text{B.20})$$

$$\begin{aligned} \frac{\partial \Psi}{\partial x_i} &= \frac{\partial}{\partial x_i} \left(\frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right] \right) \\ &= \frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \frac{\partial}{\partial x_i} \left(\exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right] \right) \\ &= \frac{\sqrt{N}}{\pi^{3/4} \sqrt{w_x w_y w_z}} \left(-\frac{1}{w_i^2} + 2i\beta_i \right) x_i \exp \left[-\frac{1}{2} \left(\frac{x^2}{w_x^2} + \frac{y^2}{w_y^2} + \frac{z^2}{w_z^2} \right) + i(x^2 \beta_x + y^2 \beta_y + z^2 \beta_z) \right]. \end{aligned}$$

Thus,

$$\begin{aligned} |\nabla\Psi(\mathbf{x}, t)|^2 &= \frac{N}{\pi^{3/2} w_x w_y w_z} \left(\frac{x^2}{w_x^4} + \frac{y^2}{w_y^4} + \frac{z^2}{w_z^4} + 4x^2 \beta_x^2 + 4y^2 \beta_y^2 + 4z^2 \beta_z^2 \right) \\ &\quad \times \exp \left[-\frac{x^2}{w_x^2} - \frac{y^2}{w_y^2} - \frac{z^2}{w_z^2} \right]. \end{aligned} \quad (\text{B.21})$$

And,

$$\int d^3\mathbf{x} \frac{\hbar^2}{2M} |\nabla\Psi(\mathbf{x}, t)|^2 = \frac{\hbar^2 N}{4M} \left(\frac{1}{w_x^2} + \frac{1}{w_y^2} + \frac{1}{w_z^2} + 4w_x^2 \beta_x^2 + 4w_y^2 \beta_y^2 + 4w_z^2 \beta_z^2 \right). \quad (\text{B.22})$$

B.2 The Euler–Lagrange Equations

As calculated in the first section, the Lagrangian of the Gaussian anzats reads:

$$\begin{aligned}
L(w_x, w_y, w_z, \beta_x, \beta_y, \beta_z) = & \frac{N\hbar}{2} \left(w_x^2 \dot{\beta}_x + w_y^2 \dot{\beta}_y + w_z^2 \dot{\beta}_z \right) \\
& + \frac{\hbar^2 N}{4M} \left(\frac{1}{w_x^2} + \frac{1}{w_y^2} + \frac{1}{w_z^2} + 4w_x^2 \beta_x^2 + 4w_y^2 \beta_y^2 + 4w_z^2 \beta_z^2 \right) \\
& + \frac{1}{4} MN \left(\omega_x^2 w_x^2 + \omega_y^2 w_y^2 + \omega_z^2 w_z^2 \right) \\
& + \frac{gN^2}{2} \frac{1}{2^{3/2} \pi^{3/2} w_x w_y w_z} \left(1 - \epsilon_{dd} F \left(\frac{w_x}{w_z}, \frac{w_y}{w_z} \right) \right) \\
& + \frac{4\sqrt{2}}{25\sqrt{5}\pi^{9/4}} \frac{N^{5/2} \gamma}{(w_x w_y w_z)^{3/2}} \\
& + 4\sqrt{2} \pi^{3/4} \theta T^2 N^{1/2} (w_x w_y w_z)^{1/2}. \tag{B.23}
\end{aligned}$$

Lagrangian per particle,

$$\frac{1}{N} L = \frac{\hbar}{2} \left(w_x^2 \dot{\beta}_x + w_y^2 \dot{\beta}_y + w_z^2 \dot{\beta}_z \right) + \frac{\hbar^2}{M} \left(w_x^2 \beta_x^2 + w_y^2 \beta_y^2 + w_z^2 \beta_z^2 \right) + G(w_x, w_y, w_z), \tag{B.24}$$

where

$$\begin{aligned}
G(w_x, w_y, w_z) = & \frac{\hbar^2}{4M} \left(\frac{1}{w_x^2} + \frac{1}{w_y^2} + \frac{1}{w_z^2} \right) + \frac{1}{4} M \left(\omega_x^2 w_x^2 + \omega_y^2 w_y^2 + \omega_z^2 w_z^2 \right) \\
& + \frac{gN}{2} \frac{1}{2^{3/2} \pi^{3/2} w_x w_y w_z} \left(1 - \epsilon_{dd} F \left(\frac{w_x}{w_z}, \frac{w_y}{w_z} \right) \right) \\
& + \frac{4\sqrt{2}}{25\sqrt{5}\pi^{9/4}} \frac{N^{3/2} \gamma}{(w_x w_y w_z)^{3/2}} + 4\sqrt{2} \pi^{3/4} \theta T^2 N^{-1/2} (w_x w_y w_z)^{1/2} \tag{B.25}
\end{aligned}$$

B.2.1 EL equations ($q \equiv w_\eta$)

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{w}_\eta} \right) - \frac{\partial L}{\partial w_\eta} = 0. \tag{B.26}$$

First, $\partial L / \partial \dot{w}_\eta = 0$, and

$$\frac{\partial(L/N)}{\partial w_\eta} = \hbar w_\eta \dot{\beta}_\eta + \frac{2\hbar^2}{M} w_\eta \beta_\eta^2 + \frac{\partial G}{\partial w_\eta} = 0. \tag{B.27}$$

B.2.2 EL equations ($q \equiv \beta_\eta$)

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\beta}_\eta} \right) - \frac{\partial L}{\partial \beta_\eta} = 0. \quad (\text{B.28})$$

First, $\frac{\partial(L/N)}{\partial \dot{\beta}_\eta} = \frac{1}{2} \hbar w_\eta^2$, then $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\beta}_\eta} \right) = \hbar w_\eta \dot{w}_\eta$. Second,

$$\frac{\partial(L/N)}{\partial \beta_\eta} = \frac{2\hbar^2}{M} w_\eta^2 \beta_\eta. \quad (\text{B.29})$$

Hence,

$$\beta_\eta = \frac{M}{2\hbar w_\eta} \dot{w}_\eta. \quad (\text{B.30})$$

B.2.3 Equation of motion for w_η

Since $\beta_\eta = \frac{M}{2\hbar w_\eta} \dot{w}_\eta$,

$$\dot{\beta}_\eta = \frac{M}{2\hbar} \left(\frac{\ddot{w}_\eta}{w_\eta} - \frac{\dot{w}_\eta^2}{w_\eta^2} \right). \quad (\text{B.31})$$

Therefore,

$$\begin{aligned} 0 &= \hbar w_\eta \frac{M}{2\hbar} \left(\frac{\ddot{w}_\eta}{w_\eta} - \frac{\dot{w}_\eta^2}{w_\eta^2} \right) + \frac{2\hbar^2}{M} w_\eta \frac{M^2}{4\hbar^2 w_\eta^2} \dot{w}_\eta^2 + \frac{\partial G}{\partial w_\eta} \\ &= \frac{M}{2} \left(\ddot{w}_\eta - \frac{\dot{w}_\eta^2}{w_\eta} \right) + \frac{M}{2} \frac{\dot{w}_\eta^2}{w_\eta} + \frac{\partial G}{\partial w_\eta}. \end{aligned}$$

Finally,

$$\frac{d^2 w_\eta}{dt^2} = -\frac{2}{M} \frac{\partial}{\partial w_\eta} G(w_x, w_y, w_z). \quad (\text{B.32})$$

We solve the equation of motion for w_η numerically, as outlined in text.