universität wien

DIPLOMARBEIT

The 2D Limit of 3D Gross-Pitaevskii Theory for Bose-Einstein Condensates

Analytical and Numerical Results

angestrebter akademischer Grad

Magister der Naturwissenschaften (Mag. rer. nat.)

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Wien, am 8. Februar 2008

"Was mich zu meiner Wissenschaft führte und von Jugend auf für sie begeisterte, ist die durchaus nicht selbstverständliche Tatsache, dass unsere Denkgesetze übereinstimmen mit den Gesetzmäßigkeiten im Ablauf der Eindrücke, die wir von der Außenwelt empfangen, dass es also dem Menschen möglich ist, durch reines Denken Aufschlüsse über jene Gesetzmäßigkeiten zu gewinnen." [1]

Max Planck

[1] Max Planck: Wissenschaftliche Selbstbiographie, Leipzig 1970, S. 8

Diese Arbeit sei meiner Familie und meinen Studienkollegen gewidmet. Sie wissen Bescheid um ihren Anteil an der erfolgreichen Fertigstellung derselben und ihre Unterstützung auf dem Weg dorthin.

Mein Dank gilt meinem Betreuer Professor Jakob Yngvason. Seine Lehre genauso wie unsere Zusammenarbeit gewährten mir tiefe Einblicke in die Physik.

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Chapter 1

Introduction

In the seventeenth century, a new era had begun in humanity's efforts to understand nature. The Aristotelian dogmata that prevailed for more than a thousand years were overcome with Galileo's *New Science*:

> "Natural philosophy is written in this grand book - I mean the universe - which stands continually open to our gaze, but it cannot be understood unless one first learns to comprehend the language in which it is written. It is written in the language of mathematics, and its characters are triangles, circles, and other geometric figures, without which it is humanly impossible to understand a single word of it."[1]

The first culmination of the scientific method came along with Newton's *Philosophiae naturalis principia mathematica*, referred to as the most significant book in the history of science. Newton's Laws and the insight that falling apples and orbiting planets are consequences of one and the same principle gave birth to a new quality in mankind's pursuit of knowledge. All authority had to be governed by experience and rationality. The following centuries witnessed the incomparable success of Newton's theory applied to the mechanical phenomena on earth and beyond. It led Laplace to the the following conclusion:

> "All events, even those which on account of their insignificance do not seem to follow the great laws of nature, are a result of it just as necessarily as the revolutions of the sun. [...] We ought then to regard the present state of the universe as the effect of its anterior state and the cause of the one which is to follow. Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective situation of the beings

[1] Galileo Galilei: Il Saggiatore, 1623

> who compose it - an intelligence sufficiently vast to submit this data to analysis - it would embrace in the same formula the movements of the greatest bodies of the universe and those of the lightest atom; for it, nothing would be uncertain and the future, as the past, would be present in its eyes."[2]

In the end of the nineteenth century it became evident that matter is made up of smallest particles, and again it were Newton's Laws, combined with statistics, that had empowered the genius of Boltzmann to describe the macroscopic behaviour of a gas based on the microscopic properties of its constituents, namely the atoms. At that time future physics was believed to be concerned merely with details:

> "The more important fundamental laws and facts of physical science have all been discovered, and these are now so firmly established that the possibility of their ever being supplanted in consequence of new discoveries is exceedingly remote... Our future discoveries must be looked for in the sixth place of decimals."[3]

But within a few years, several observations revealed that the most fundamental principles underlying all natural processes have to obey rules of a totally different kind.

The development of quantum mechanics in an explosion of creativity in the first half of the twentieth century marked the most dramatic revolution of the foundations of physics since the days of Newton. It provided the theoretical framework to correctly describe nature on a microscopic level, but the conclusions drawn from its interpretation posed highly philosophical questions. One of the remarkable consequences is that reality can no longer be treated independently from its observer:

> "Man lehrte die Generation, zu der Einstein, Bohr und ich gehören, daß eine objektive physikalische Welt existiert, die sich nach unveränderlichen Gesetzen entfaltet, die von uns unabhängig sind. Wir betrachten diesen Vorgang, wie das Publikum im Theater ein Stück verfolgt. [...] Die Quantenmechanik deutet indessen die in der Atomphysik gewonnene Erfahrung auf eine andere Weise. Wir können den Beobachter einer physikalischen Erscheinung nicht mit dem Publikum bei einer Theateraufführung vergleichen, sondern eher mit dem bei einem Fußballspiel [...] Ein noch besseres Gleichnis ist das Leben selbst, wo Publikum und Akteure die gleichen Personen sind."[4]

[2] Pierre-Simon Laplace: Essay on Probabilities, 1814
[3] Albert A. Michelson: Speech at the dedication of Ryerson Physics Lab, U. of Chicago 1894
[4] Max Born: Physik im Wandel meiner Zeit. Vieweg, Braunschweig 1966

All predictions dealing with microscopic physical systems are of a probabilistic kind. Single events, such as the decay of a radioactive atom, are in principle not determined. Moreover, it became clear that our language is not capable of expressing the observed phenomena without ending up in contradictions. It depends indeed on the question we ask in an experiment if one and the same object under consideration behaves like a wave or like a particle - which is of course completely opposed to all our logical tradition. This duality of matter and waves is expressed mathematically by the de Broglie relation: to every particle of mass m and energy E corresponds a wavelength λ_{dB}, given by

$$\lambda_{\mathrm{dB}} = \frac{h}{\sqrt{2mE}}, \tag{1.1}$$

with Planck's constant h. However, despite all these difficulties, it was possible - due to the remarkable intuition of physicists like Heisenberg and Schrödinger - to find this abstract mathematical theory of quantum mechanics, whose results perfectly mirror the experimental observations.

Quantum mechanics also provided the basis to describe systems of many particles, such as gases, from a new point of view. It turned out that all quantum mechanical objects can be distinguished by an intrinsic property known as the *spin*. Particles having integer spin, referred to as bosons, obey a different statistics than fermions, i. e. particles with half-integer spin. It is this statistics which dramatically influences the behaviour of physical systems. On the one hand, Pauli's exclusion principle says that a given quantum state can be occupied by a single fermion only. A consequence of this is the "orbital" structure of atoms, devoted to the fact that the electron has spin 1/2. Moreover, it is the reason why atoms are stable at all. For bosons, on the other hand, there is no such limitation on the occupation number of quantum states. While at high temperatures bosonic systems behave like classical gases, their quantum character becomes more and more apparent as the temperature tends to absolute zero. To see this, remember that the energy of a free particle is proportional to the temperature, i. e. $E \sim k_B T$, with k_B Boltzmann's constant. Then, as the temperature gets lower, the de Broglie wavelength (1.1) may become comparable and even larger than the mean particle distance. The classical picture of a gas made up of single particles then completely fails, but it may be thought of a system of overlapping matter waves that finally, as the temperature approaches zero, constitutes a macroscopic quantum object. This is the phenomenon we refer to as Bose-Einstein condensation. For non-interacting gases its occurrence was demonstrated by Einstein in 1925 [12], based on the statistics of spinless particles derived by Bose [6]. But it was only 70 years later that Bose-Einstein Condensation (BEC) was realized experimentally for the first time [1].

Nevertheless, in these decades many advances were achieved in the understanding of Bose gases at low temperatures. A first cornerstone marked F. London's suggestion in 1938 [25] that superfluid liquid helium might be a manifestation of BEC. However, this system is - due to its strong interactions - far away from being an ideal gas, and thus cannot be understood by means of Einstein's theory. Bogoliubov's seminal analysis from 1947 [5] then significantly contributed to the theory of the bosonic many-body problem, but the first mathematically rigorous results date back to the 50's and 60's. Dyson could establish an asymptotically correct upper bound on the ground state energy of hard-core bosons in 1957 [9], while Lieb and Liniger [18] investigated exactly solvable models of one-dimensional Bose gases in 1963. An important extension was Schick's energy formula for a two-dimensional system [28], that was proved rigorously 30 years later [24]. In 1961, Gross and Pitaevskii independently derived an equation when investigating vortices in Bose gases [15, 27]. The importance of this so called Gross-Pitaevskii equation for the study of dilute Bose gases was pointed out by Baym and Pethick [4], who showed that it adequately describes Bose-Einstein condensates as studied in the first experiments. On the experimental side, much progress has been made since 1995. We want to particularly emphasize that by magneto-optical trapping with strong confinement in one or two directions, it has been possible to create systems that are essentially lower dimensional [13, 14, 16]. The theoretical investigations in Chapters 3ff of the present work in fact will deal with these configurations.

In the last 10 years, many of the properties of Bose gases proposed in the 50's and 60's could also be proved rigorously. The following chapter accounts for some of the advances made in this field.

Chapter 2

Mathematical Approach to the Bose Gas and Bose-Einstein Condensation

In this chapter we want to recall some fundamental results on the theory of the Bose gas and Bose-Einstein condensation. This enables us to understand the basic concepts underlying the main part of this work, namely the behaviour of a Bose condensate in the limit from 3D to 2D, which will be discussed in Chapter 3.

Every analysis of the bosonic many-particle problem has to start with specifying the Hamiltonian appropriate for the system under consideration. One can then seek to derive ground state properties, e. g. for the energy and density. Furthermore, in a particular situation known as the Gross-Pitaevskii limit, even the occurrence of Bose-Einstein condensation can be demonstrated.

All the facts presented here, including the full proofs, are discussed in the monograph [20].

2.1 The Homogeneous Bose Gas

The first model we want to investigate is the homogeneous Bose gas in three dimensions, i. e. a system of N identical bosons in a cubic box of side length L, that interact via a radially symmetric, repulsive pair potential v that is assumed to be nonnegative and of finite range. Thus, the Hamiltonian H_N, operating on symmetric wave functions, reads

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|). \tag{2.1}$$

Units are chosen such that $\hbar = 2m = 1$. Now the main quantity of interest is the ground state energy, defined by

$$E_0(N, L) = \inf_{\psi} \frac{\langle \psi, H_N \psi \rangle}{\langle \psi, \psi \rangle}, \tag{2.2}$$

and its thermodynamic limit, which is obtained by letting $L \to \infty$ while keeping the density $\rho = N/L^3$ constant. In this limit, the energy per particle reads

$$e_0(\rho) = \lim_{L \to \infty} \frac{E_0(\rho L^3, L)}{\rho L^3}. \tag{2.3}$$

We are particularly interested in the case of low densities, as this reflects the experimental settings. This means we consider the situation in which the mean particle distance $\rho^{-1/3}$ is large compared to the *scattering length* a associated with the potential v and determining the range and strength of the interaction. a is defined via the solution of the zero energy scattering equation

$$(-2\Delta + v(|\mathbf{x}|))\, \psi_0 = 0. \tag{2.4}$$

If $v(|\mathbf{x}|) = 0$ for $|\mathbf{x}| > R_0$, ψ_0 satisfies (after normalization) $\psi_0(\mathbf{x}) = 1 - a/|\mathbf{x}|$ for all $|\mathbf{x}| > R_0$, and this defines a.

Now the formula for the ground state energy per particle that was 'known' for several decades, but proved only recently, is

$$e_0(\rho) \approx 4\pi\rho a \tag{2.5}$$

for low densities, i. e. $\rho a^3 \ll 1$. It can be made plausible by the following heuristics, which goes essentially back to a paper of W. Lenz from 1929 [17]. Consider a system of two particles and calculate the energy of the zero energy scattering solution ψ_0 in a ball of radius R. Partial integration of (2.4) yields

$$\int_{|\mathbf{x}| \leq R|} \left\{ 2|\nabla \psi_0|^2 + v|\psi_0|^2 \right\} d^3x = 8\pi a \left(1 - \frac{a}{R}\right) \to 8\pi a \quad \text{for } R \to \infty. \tag{2.6}$$

The same holds true for a box with side length L, if $L \to \infty$. Dividing by the normalization gives the energy of this pair of particles, namely $8\pi a/L^3$. For a system of N particles, we have $N(N-1)/2 \approx N^2/2$ pairs, and considering them independent we can sum up all these contributions, which gives

$$E_0(N, L) \approx 4\pi N^2 a/L^3 = 4\pi N \rho a. \tag{2.7}$$

In the thermodynamic limit, this equals expression (2.5).

This simple heuristics is not a proof of (2.5), however, because the ground state wave function could have subtle correlations rendering the assumption of independent pairs invalid. In fact, the corresponding argument in two dimensions gives a wrong answer, as will be discussed in Section 2.3. But (2.5) can

indeed be proved rigorously. The main step was the lower bound achieved in 1998 by E. Lieb and J. Yngvason [23]. The upper bound was established already in 1957 by F. Dyson [9] (for hard core bosons) and generalized by R. Seiringer [30] to arbitrary (positive) short range interactions, see also [31]. The precise result of [23] is the following

Theorem 1

$$\lim_{\rho a^3 \to \infty} \frac{e_0(\rho)}{4\pi\rho a} = 1. \tag{2.8}$$

Now we want to present the main ideas underlying the proof of this last theorem. Of course, one has to establish upper and lower bounds on the energy. For the upper bound, one defines a so-called *Dyson wave function* $F(\mathbf{x}_1, ...\mathbf{x}_N)$, which basically is a product of two-particle wave functions $f_i(\mathbf{x}_i, \mathbf{x}_j)$, where $\mathbf{x}_j$ marks the nearest neighbour of $\mathbf{x}_i$. Although F is not symmetric, it may be used as a trial function for an upper bound, as the absolute ground state of (2.1) is symmetric. With this ansatz one can evaluate $\langle\psi, H_N\psi\rangle/\langle\psi,\psi\rangle$ to get the expected estimate from above on the energy, with errors that vanish as the density parameter $Y = 4\pi\rho a^3/3$ tends to zero.

As one might expect, the lower bound is more complicated. In a first step, by a lemma of Dyson [9] a 'hard' potential can be substituted by a 'soft' one, sacrificing the kinetic energy. More precisely, with v as in (2.4) and $|\mathbf{x}| \equiv r$, for any function $U(r)$ satisfying $\int U(r)r^2dr \leq 1$ and $U(r) = 0$ for $r < R_0$, the lemma says that

$$\int_{\mathcal{B}} \left(|\nabla\psi|^2 + (v/2)|\psi|^2\right) d^3x \geq a \int_{\mathcal{B}} U|\psi|^2 d^3x, \tag{2.9}$$

for $\mathcal{B} \subset \mathbb{R}^3$ convex. By this means, Dyson derived a lower bound for a hard core gas of bosons [9], which is, however, about 14 times too small. In [23] the correct bound was proved by keeping a small amount of the kinetic energy in the Hamiltonian, i. e. by writing

$$H_N = \epsilon H_N + (1-\epsilon)H_N \geq \sum_i \epsilon\Delta_i + (1-\epsilon)H_N \tag{2.10}$$

and applying Dyson's lemma to the second part of this last expression only. Then, using first-order perturbation theory, one can calculate the expectation value, while Temple's inequality (3.15) allows us to control the error term. As a consequence, to keep the error constant in the thermodynamic limit, space must be divided into small boxes with fixed side length. The N particles are then distributed among these cells, and minimizing over all possible choices of the particle numbers for the various cells leads to a lower bound. The result, which - together with the upper bound - proves Theorem 1 in the low density limit, is

$$\frac{e_0(\rho)}{4\pi a\rho} \geq 1 - CY^{1/17}. \tag{2.11}$$

2.2 Inhomogeneous Systems and Gross-Pitaevskii Theory

2.2.1 The Hamiltonian

Again we consider a system of N identical bosons, but now we add an external potential V to the Hamiltonian:

$$H_N = \sum_{i=1}^{N} (-\Delta_i + V(\mathbf{x}_i)) + \sum_{1 \le i < j \le N} v(|\mathbf{x}_i - \mathbf{x}_j|), \tag{2.12}$$

where V is assumed to tend to infinity as $|\mathbf{x}| \to \infty$. We measure energies in units of the ground state energy of the operator $-\Delta + V(\mathbf{x})$, say $\hbar\omega$. The oscillator length $a_{osc} = \sqrt{\hbar/m\omega}$ associated with the trapping potential provides a natural length scale, measuring the extension of the gas cloud. We denote the lowest energy of the Hamiltonian (2.12) by $E^{\mathrm{Q}}_{\mathrm{3D}}(N, a)$, as the relevant parameters are the particle number N and the scattering length a (see Section 2.1). It is defined, for symmetric wave functions ψ, as

$$E^{\mathrm{Q}}_{\mathrm{3D}}(N, a) := \inf_{\psi} \frac{\langle \psi, H_N \psi \rangle}{\langle \psi, \psi \rangle}. \tag{2.13}$$

A quantum mechanical N-body problem of this kind is, as presented in the previous section, a very subtle affair. However, under certain circumstances, things can be substantially simplified, as we shall see in the next section.

2.2.2 Gross-Pitaevskii Theory

We begin by defining the Gross-Pitaevskii (GP) energy functional [15, 27] for the one-particle wave function $\phi(\mathbf{x})$:

$$\mathcal{E}^{\mathrm{GP}}_{\mathrm{3D}}[\phi] = \int_{\mathbb{R}^3} \left\{ |\nabla\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + 4\pi a |\phi(\mathbf{x})|^4 \right\} d^3x. \tag{2.14}$$

It can be shown (see e. g. [21]) that under the normalization condition $\int |\phi(\mathbf{x})|^2 d^3x = N$ there exists a unique ϕ^{GP} which minimizes the functional (2.14). Thus we can introduce the GP energy as

$$E^{\mathrm{GP}}_{\mathrm{3D}}(N, a) := \inf \left\{ \mathcal{E}^{\mathrm{GP}}_{\mathrm{3D}}[\phi] : \int |\phi(\mathbf{x})|^2 d^3x = N \right\} = \mathcal{E}^{\mathrm{GP}}_{\mathrm{3D}}[\phi^{\mathrm{GP}}]. \tag{2.15}$$

Setting $\psi = N^{1/2}\phi$ one can easily verify that it satisfies a simple scaling relation:

$$E^{\mathrm{GP}}_{\mathrm{3D}}(N, a) = N E^{\mathrm{GP}}_{\mathrm{3D}}(1, Na). \tag{2.16}$$

A variational calculation shows that associated with the energy functional (2.14) is the GP equation for the normalized minimizer ϕ^{GP}, which reads

$$-\Delta\phi^{\mathrm{GP}} + V\phi^{\mathrm{GP}} + 8\pi a|\phi^{\mathrm{GP}}|^2\phi^{\mathrm{GP}} = \mu\phi^{\mathrm{GP}}. \tag{2.17}$$

The parameter μ is the chemical potential, given by

$$\mu = \frac{dE_{\mathrm{3D}}^{\mathrm{GP}}(N,a)}{dN} = E_{\mathrm{3D}}^{\mathrm{GP}}(N,a)/N + 4\pi Na\int |\phi|^4 d^3x. \tag{2.18}$$

The Gross-Pitaevskii equation is also the starting point for numerical calculations on Bose-Einstein condensates, as we shall see in Chapter 4.

Now what has GP theory to do with the many-body problem posed in Section 2.2.1? The astonishing fact is that there is indeed a definite correspondence of the Hamiltonian (2.12) and the GP energy functional: Consider the limit $N \to \infty$, while keeping the parameter Na fixed. In this case, referred to as the Gross-Pitaevskii limit, the GP energy (2.15) converges to the quantum mechanical ground state energy (2.13):

Theorem 2 *If $N \to \infty$ with Na fixed, then*

$$\lim_{N\to\infty} \frac{E_{\mathrm{3D}}^{\mathrm{Q}}(N,a)}{E_{\mathrm{3D}}^{\mathrm{GP}}(N,a)} = 1. \tag{2.19}$$

A rigorous proof of this theorem, based on the results on the homogeneous Bose gas of Section 2.1, was given in [21]. Now the seemingly particular limit of GP theory is not only of academic interest. In fact, experiments on Bose-Einstein condensates feature the same characteristics. To see this, take the dimensionless version of the GP limit, i. e. take $N \to \infty$ with $Na/a_{\mathrm{osc}} = \mathrm{const}$. As a consequence,

$$\rho a^3 \sim \frac{Na^3}{a_{\mathrm{osc}}^3} = \frac{1}{N^2}\left(\frac{Na}{a_{\mathrm{osc}}}\right)^3 \to 0. \tag{2.20}$$

Thus we see that the GP case is a thermodynamic limit combined with a limit of low densities, reflecting the typical experimental situation when studying dilute Bose gases.

2.2.3 Bose-Einstein Condensation in the GP Limit

So far we have said nothing about the occurrence of Bose-Einstein Condensation. In fact, for the homogeneous system discussed in Section 2.1, there is no proof of BEC in the usual thermodynamic limit available by now. But, as we shall see, the situation is different for the Gross-Pitaevskii limit.

Now what do we mean by Bose-Einstein condensation in the case of an interacting gas? To clarify this, consider the normalized ground state wave

function Ψ_0 of the Hamiltonian (2.12). Then the corresponding one-particle density matrix is defined as

$$\gamma_N(\mathbf{x},\mathbf{x}') = N\int \Psi_0(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_N)\bar{\Psi}_0(\mathbf{x}',\mathbf{x}_2,\ldots,\mathbf{x}_N)d\mathbf{x}_2\ldots d\mathbf{x}_N. \qquad (2.21)$$

Thus γ_N is a positive trace class operator on $L^2(\mathbb{R}^3,d\mathbf{x})$, with $\mathrm{Tr}\,\gamma_N = N$. Denote the eigenvalues of γ_N in decreasing order by λ_ν, $\nu = 0,1,\ldots$ and interpret them as occupation numbers of the corresponding eigenstates. Now we can give a precise definition of BEC, following [26]: *Bose-Einstein condensation in the ground state means that the eigenvalue λ_0 is of order N as $N\to\infty$.* In other words, the ground state is macroscopically occupied if $\lambda_0 \geq CN$ for $N\to\infty$ with some positive constant C independent of N. *Complete* BEC means that $\lambda_0/N \to 1$ as $N\to\infty$.

The rigorous result proved in [19] by E. H. Lieb and R. Seiringer in 2002 is the following:

Theorem 3 *Let γ_N be the one-particle density matrix of the ground state of H_N and denote by ϕ^{GP} the unique, normalized minimizer of $\mathcal{E}^{\mathrm{GP}}_{3\mathrm{D}}$. Then, if $N\to\infty$ with Na fixed,*

$$\mathrm{Tr}\left|\frac{1}{N}\gamma_N - |\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}|\right| \to 0. \qquad (2.22)$$

This last theorem states that in the GP limit complete Bose-Einstein condensation occurs in the ground state. Moreover, the eigenfunction of γ_N with the largest eigenvalue is indeed given by GP theory as $N\to\infty$. For this reason, ϕ^{GP} is referred to as the 'condensate wave function'.

2.3 The Bose Gas in Two Dimensions

The questions we have discussed in Sections 2.1 and 2.2 on the Bose gas in three-dimensional space can be analogously investigated for bosons in a two-dimensional plane. For the homogeneous case, it was proved [24] that the ground state energy is given by $4\pi\rho_{2\mathrm{D}}/|\ln(\rho_{2\mathrm{D}}a_{2\mathrm{D}}^2)|$, with $\rho_{2\mathrm{D}}$ and $a_{2\mathrm{D}}$ the 2D density and scattering length, respectively. Thus the result cannot be interpreted as the sum over the energies of independent pairs as in 3D (see Section 2.1), it is indeed much bigger.

Nevertheless, for inhomogeneous systems in 2D a Gross-Pitaevskii theory of the same kind as presented in Section 2.2.2 can be derived [22]. It is based on the 2D energy functional

$$\mathcal{E}^{\mathrm{GP}}_{2\mathrm{D}}[\varphi] = \int_{\mathbb{R}^2}\left\{|\nabla\varphi(x)|^2 + V(x)|\varphi(x)|^2 + 4\pi g|\varphi(x)|^4\right\}d^2x, \qquad (2.23)$$

with $x \in \mathbb{R}^2$. The only difference to the 3D case is the coupling parameter, which can be taken to be $g \sim |\ln(\bar{\rho}a_{\mathrm{2D}}^2)|^{-1}$, with a mean density $\bar{\rho}$ to be defined more precisely later (3.6). As in Section 2.2.2 we introduce the GP energy by writing

$$E_{\mathrm{2D}}^{\mathrm{GP}}(N,g) = \inf\left\{\mathcal{E}_{\mathrm{2D}}^{\mathrm{GP}}[\varphi] : \int |\varphi(x)|^2 d^2x = N\right\}. \tag{2.24}$$

In Chapter 3 we will consider disk-shaped condensates, realized by a three-dimensional trap that is strongly confining in one spatial direction. Then one can distinguish between two different parameter regimes, characterized by the form of the coupling constant g. Denote the 'thickness' of the condensate by h, and let a be the 3D scattering length. Then, in the region $a/h \ll |\ln(\bar{\rho}h^2)|^{-1}$, which will be relevant for the forthcoming chapter, the coupling parameter for the 2D energy functional is $\sim a/h$ (see [29] for details). In this case we shall show that there exists a well defined correspondence between the 3D and 2D Gross-Pitaevskii theories.

Chapter 3

Disk-Shaped Bose-Einstein Condensates

Based on the theoretical framework presented previously we now establish relations between the 3D and 2D theories. More precisely, we investigate the physical situation, where a trapped 3D BEC suffers an increasing confinement in one spatial direction, and hence becomes effectively two-dimensional [13, 14]. The question we address here is the following: Can this transition be understood and expressed in terms of GP theory? And does it yield the 2D GP theory that was derived from the 2D many-body problem in [29]? For a certain parameter regime, the answer is yes.

3.1 Preliminaries - The Setting

The relevant physical quantities we shall compare are the GP energies in the 3D and 2D cases, denoted by $E^{\mathrm{GP}}_{\mathrm{3D}}(N, L, h, a)$ and $E^{\mathrm{GP}}_{\mathrm{2D}}(N, L, g)$, respectively. As we have seen previously, they are obtained by minimizing the corresponding energy functionals (2.14) and (2.23). Taking into account the special setting of the problem, we introduce the following conventions and notations. Consider a trapping potential confining strongly in z-direction and denote its 'thickness' by h. We identify h with the oscillator length a_z in this direction, and therefore have $h \sim \omega_z^{-1/2}$, ω_i being the frequency associated with the potential in i-th direction. As in Chapter 2, a is the 3D scattering length, and points $\mathbf{x} \in \mathbb{R}^3$ are written as (x, z), $x \in \mathbb{R}^2$, $z \in \mathbb{R}$. The Hamiltonian for N identical bosons then is

$$H_{N,L,h,a} = \sum_{i=1}^{N} \left(-\Delta_i + V_{L,h}(\mathbf{x}_i)\right) + \sum_{1 \le i < j \le N} v_a(|\mathbf{x}_i - \mathbf{x}_j|). \tag{3.1}$$

Here $V_{L,h}$ and v_a are the confining and interaction potentials, respectively,

with the scaling

$$V_{L,h}(\mathbf{x}) = V_L(x) + V_h^\perp(z) = \frac{1}{L^2}V(L^{-1}x) + \frac{1}{h^2}V^\perp(h^{-1}z), \tag{3.2}$$

$$v_a(|\mathbf{x}|) = \frac{1}{a^2}v(a^{-1}|\mathbf{x}|). \tag{3.3}$$

For V, $V^\perp$ and v fixed we have L, h and a as scaling parameters, keeping in mind the scaling relation (2.16) for the 3D GP energy per particle, which now reads

$$E_{\rm 3D}^{\rm GP}(N, L, h, a)/N = (1/L^2)E_{\rm 3D}^{\rm GP}(1, 1, h/L, Na/L). \tag{3.4}$$

For the 2D GP energy, one has

$$E_{\rm 2D}^{\rm GP}(N, L, g) = (N/L^2)E_{\rm 2D}^{\rm GP}(1, 1, Ng). \tag{3.5}$$

Taking the normalized minimizer $\varphi_{Ng}^{\rm GP}$ of the 2D energy functional (2.23), we can define a mean density by

$$\bar{\rho}_{Ng} = N\int |\varphi_{Ng}^{\rm GP}|^4. \tag{3.6}$$

The link between $E_{\rm 3D}^{\rm GP}$ and $E_{\rm 2D}^{\rm GP}$ is, as we shall see, the confining one-particle energy in z-direction, $e^\perp$, of the potential $V^\perp$. It corresponds to the ground state $s(z)$ of the one-particle Hamiltonian $-d^2/dz^2 + V^\perp(z)$. Then, writing $s_h(z) = h^{-1/2}s(h^{-1}z)$ and $V_h^\perp(z) = h^{-2}V^\perp(h^{-1}z)$ as in (3.2) we get $e_h^\perp = h^{-2}e^\perp$ as lowest eigenvalue of $-d^2/dz^2 + V_h^\perp(z)$:

$$\begin{aligned} e^\perp &= \int \left[(\partial_z s(z))^2 + V^\perp(z)s(z)^2\right] dz \\ &= \int \left[h^2(\partial_{z'} s(h^{-1}z'))^2 + V^\perp(h^{-1}z')s(h^{-1}z')^2\right] h^{-1}dz' \\ &= \int \left[h^3(\partial_{z'} s_h(z'))^2 + h^3 V_h^\perp(z')s_h(z')^2\right] h^{-1}dz' \\ &= h^2 e_h^\perp \end{aligned}$$

Now we have collected all the prerequisites to state the precise theorem.

3.2 Theorem for the 2D Limit of 3D GP Theory

Theorem 4 *Define* $g = (\int s(z)^4 dz)a/h$. *If* $h/L \to 0$, *then*

$$\frac{E_{\rm 3D}^{\rm GP}(N, L, h, a) - Nh^{-2}e^\perp}{E_{\rm 2D}^{\rm GP}(N, L, g)} \to 1 \tag{3.7}$$

uniformly in the parameters, as long as $\bar{\rho}ah \to 0$.

Remarks. The parameter regime we are concerned with is characterized by the fact that the 2D coupling g can be set $\sim a/h$. Consequently, the condition $\bar{\rho}ah \to 0$ is equivalent to $h^2\bar{\rho}g \to 0$, which simply means that the confining energy $\sim h^{-2}$ is much larger than the internal energy $\bar{\rho}g$. Furthermore, the following observation is useful for proving the theorem and estimating the errors. In the energy functional (2.23), the gradient term as well as the potential term are $\sim 1/L^2$, whereas the interaction term is $\bar{\rho}g$. So $E^{\rm GP}_{\rm 2D}(1, L, Ng) \sim L^{-2} + \bar{\rho}a/h$ and we conclude that

$$\bar{\rho}ah \to 0 \text{ if and only if } h^2 E^{\rm GP}_{\rm 2D}(1, L, Ng) \to 0. \tag{3.8}$$

Proof of Theorem 4. The proof is essentially taken from [29]. Here we extend it to investigate the functional behaviour of the errors. Because of the scaling relation (3.4) it suffices to deal with the case $N = 1$ and $L = 1$.

i. Upper bound on the 3D GP energy

The upper bound is obtained by evaluating the energy functional $\mathcal{E}^{\rm GP}_{\rm 3D}[\phi]$ for the trial function ϕ defined as

$$\phi(\mathbf{x}) = \varphi_{\rm GP}(x) s_h(z) \quad x \in \mathbb{R}^2, z \in \mathbb{R}. \tag{3.9}$$

Here $\varphi_{\rm GP}(x)$ is the normalized minimizer of the 2D GP functional and s_h the normalized ground state wave function of $-d^2/dz^2 + V_h^{\perp}(z)$. Then, with $V_{1,h}(\mathbf{x}) = V_1(x) + V_h^{\perp}(z)$, one has

$$\begin{aligned}
\mathcal{E}^{\rm GP}_{\rm 3D}[\phi] &= \int \{|\nabla\phi(\mathbf{x})|^2 + V_{1,h}(\mathbf{x})|\phi(\mathbf{x})|^2 + 4\pi a|\phi(\mathbf{x})|^4\} d^3x \\
&= \int \{s_h(z)^2 |\nabla_x \varphi_{\rm GP}(x)|^2 + s_h(z)^2 |\varphi_{\rm GP}(x)|^2 V_1(x) + 4\pi a s_h(z)^4 |\varphi_{\rm GP}(x)|^4\} d^3x \\
&+ \int \{|\varphi_{\rm GP}(x)|^2 (\partial_z s_h(z))^2 + V_h(z)|\varphi_{\rm GP}(x)|^2 s_h(z)^2\} d^3x \\
&= \int \{|\nabla_x \varphi_{\rm GP}(x)|^2 + |\varphi_{\rm GP}(x)|^2 V_1(x) + 4\pi g |\varphi_{\rm GP}(x)|^4\} dx \\
&+ \int \{(\partial_z s_h(z))^2 + V_h(z) s_h(z)^2\} dz \\
&= E^{\rm GP}_{\rm 2D}(1, 1, g) + e^{\perp}/h^2,
\end{aligned}$$

where we have used that $\varphi_{\rm GP}$ and s_h are normalized and

$$a \int s_h(z)^4 dz = a \int h^{-2} s(h^{-1}z)^4 dz = (a/h) \int s(z')^4 dz' \equiv g. \tag{3.10}$$

Hence we have the upper bound

$$E^{\mathrm{GP}}_{\mathrm{3D}}(1,1,h,a) \leq \mathcal{E}^{\mathrm{GP}}_{\mathrm{3D}}[\phi] = e^{\perp}/h^2 + E^{\mathrm{GP}}_{\mathrm{2D}}(1,1,g). \tag{3.11}$$

ii. Lower bound on the 3D GP energy

In a first step we consider the one-particle Hamiltonian

$$H_{h,a} = -\Delta + V_{1,h}(\mathbf{x}) + 8\pi a|\varphi_{\mathrm{GP}}(x)|^2 s_h(z)^2. \tag{3.12}$$

Using the minimizer Φ of the 3D GP functional as a test state for $H_{h,a}$ yields

$$\begin{aligned}
\text{infspec } H_{h,a} &\leq \langle \Phi, H_{h,a}\Phi\rangle \\
&= E^{\mathrm{GP}}_{\mathrm{3D}}(1,1,h,a) - 4\pi a \int_{\mathbb{R}^3} |\Phi(\mathbf{x})|^4 dx \\
&+ 8\pi a \int |\varphi_{\mathrm{GP}}(x)|^2 s_h(z)^2 |\Phi(\mathbf{x})|^2 d^3x \\
&\leq E^{\mathrm{GP}}_{\mathrm{3D}}(1,1,h,a) + 4\pi a \int_{\mathbb{R}^3} |\varphi_{\mathrm{GP}}(x)|^4 s_h(z)^4 d^3x \\
&= E^{\mathrm{GP}}_{\mathrm{3D}}(1,1,h,a) + 4\pi g \int_{\mathbb{R}^2} |\varphi_{\mathrm{GP}}(x)|^4 dx.
\end{aligned} \tag{3.13}$$

The last inequality follows from $2\int fg \leq (\int f^2 + \int g^2)$.

In the next step, we split the Hamiltonian (3.12) into a two-dimensional and a one-dimensional part, the latter, for fixed $x \in \mathbb{R}^2$, being

$$H_{h,a,x} = -\partial_z^2 + V_h^{\perp}(z) + 8\pi a|\varphi_{\mathrm{GP}}(x)|^2 s_h(z)^2. \tag{3.14}$$

.

Now this operator (3.14) can be bounded from below using Temple's inequality [32], which says that for any Hamiltonian H with lowest eigenvalues $E_0 < E_1$ and expectation value $\langle H\rangle < E_1$ in some state,

$$E_0 \geq \langle H\rangle - \frac{\langle (H - \langle H\rangle)^2\rangle}{E_1 - \langle H\rangle}. \tag{3.15}$$

We apply this to $H = H_{h,a,x}$ and the ground state s_h of the free part $-\partial_z^2 + V_h^{\perp}(z)$. Due to the positivity of the perturbation $8\pi a|\varphi_{\mathrm{GP}}(x)|^2 s_h(z)^2$ we have $E_1 \geq \tilde{e}^{\perp}/h^2$, where $\tilde{e}^{\perp}$ is the lowest eigenvalue above the ground state energy of $-\partial_z^2 + V^{\perp}(z)$. Hence, Temple's inequality gives

$$H_{h,a,x} \geq \langle H_{h,a,x}\rangle\,(1 - \delta_{\mathrm{T}}) \tag{3.16}$$

with the expectation value $\langle H_{h,a,x}\rangle$ and the error term δ_{T} given by

$$\langle H_{h,a,x}\rangle = e^{\perp}/h^2 + 8\pi g|\varphi_{\mathrm{GP}}(x)|^2 \tag{3.17}$$

$$\delta_{\mathrm{T}} = \frac{\langle (H_{h,a,x} - \langle H_{h,a,x}\rangle)^2\rangle}{\langle H_{h,a,x}\rangle(\tilde{e}^{\perp}/h^2 - \langle H_{h,a,x}\rangle)}. \tag{3.18}$$

Lemma 1 *The error term in Temple's inequality tends to zero in the above limit, more precisely,* $\delta_{\mathrm{T}} = O(h^4 E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)^2)$.

Proof of Lemma 1. To calculate the denominator, we see from (3.14) that

$$H_{h,a,x} s_h = (h^{-2} e^{\perp}) s_h + 8\pi a |\varphi_{\mathrm{GP}}(x)|^2 s_h^3 \tag{3.19}$$

and therefore (by (3.17))

$$\left(H_{h,a,x} - \langle H_{h,a,x}\rangle\right) s_h = 8\pi a |\varphi_{\mathrm{GP}}(x)|^2 (a s_h^3 - g s_h). \tag{3.20}$$

Taking into account that

$$\int (a s_h(z)^3 - g s_h(z))^2 dz = (a/h)^2 \left[\int s^6 - \left(\int s^4\right)^2\right] \tag{3.21}$$

we get

$$\begin{aligned} \langle (H_{h,a,x} - \langle H_{h,a,x}\rangle)^2\rangle &= (8\pi)^2 |\varphi_{\mathrm{GP}}(x)|^4 \int \left(a s_h(z)^3 - g s_h(z)\right)^2 dz \\ &\leq (8\pi)^2 \|\varphi_{\mathrm{GP}}\|_\infty^4 (a/h)^2 \left[\int s^6 - \left(\int s^4\right)^2\right] \end{aligned} \tag{3.22}$$

When comparing these analytic estimates to numerical calculations, we will explicitly evaluate this last term (c. f. equation (5.3) in Section 5).

Now, by Lemma 2.1 in [22], $8\pi g \|\varphi_{\mathrm{GP}}\|_\infty^2$ can be bounded by the chemical potential μ^{GP} and thus by const.$E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)$:

$$\langle (H_{h,a,x} - \langle H_{h,a,x}\rangle)^2\rangle \leq \text{const.} E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)^2 = O(E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)^2). \tag{3.23}$$

For the numerator, we estimate

$$\begin{aligned} \langle H_{h,a,x}\rangle \left(\tilde{e}^{\perp}/h^2 - \langle H_{h,a,x}\rangle\right) &\geq e^{\perp}/h^2 \left((\tilde{e}^{\perp} - e^{\perp})/h^2 - 8\pi g |\varphi_{\mathrm{GP}}(x)|^2\right) \\ &\geq e^{\perp}(\tilde{e}^{\perp} - e^{\perp})/h^4 \left(1 - (8\pi/(\tilde{e}^{\perp} - e^{\perp})) h^2 g \|\varphi_{\mathrm{GP}}\|_\infty^2\right) \\ &\geq \text{const.}/h^4 \left(1 - \text{const.} h^2 E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)\right). \end{aligned} \tag{3.24}$$

Combining (3.23) and (3.24) we find for the error term

$$\begin{aligned} \delta_{\mathrm{T}} &\leq \frac{\text{const.} h^4 E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)^2}{1 - \text{const.} h^2 E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)} \\ &= \text{const.} h^4 E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g)^2 \left(1 + O(h^2 E_{\mathrm{2D}}^{\mathrm{GP}}(1,1,g))\right). \end{aligned} \tag{3.25}$$

◇

For the operator (3.12) we can write $H_{h,a} = -\Delta_x + V(x) + H_{h,a,x}$, which, by equation (3.16), has a lower bound

$$H_{h,a} \geq -\Delta_x + V(x) + (e^{\perp}/h^2 + 8\pi g|\varphi_{\mathrm{GP}}(x)|^2)(1 - \delta_{\mathrm{T}}). \tag{3.26}$$

Now the lowest energy of $-\Delta_x + V(x) + 8\pi g|\varphi_{\mathrm{GP}}(x)|^2$ is just $E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g) + 4\pi g \int_{\mathbb{R}^2} |\varphi_{\mathrm{GP}}(x)|^4 dx$, so from (3.13) and (3.26) we conclude that

$$E^{\mathrm{GP}}_{3\mathrm{D}}(1,1,h,a) \geq E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g) + e^{\perp}/h^2 - (e^{\perp}/h^2 + 8\pi g\|\varphi_{\mathrm{GP}}\|^2_{\infty})\delta_{\mathrm{T}} \tag{3.27}$$

or equivalently

$$\frac{E^{\mathrm{GP}}_{3\mathrm{D}}(1,1,h,a) - e^{\perp}/h^2}{E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g)} \geq 1 - \Delta e. \tag{3.28}$$

For the error term Δe of the limit theorem we have, using Lemma 1 and $g\|\varphi_{\mathrm{GP}}\|^2_{\infty} \sim E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g)$,

$$\Delta e = \frac{e^{\perp} + 8\pi h^2 g\|\varphi_{\mathrm{GP}}\|^2_{\infty}}{h^2 E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g)} \cdot \mathrm{const.} h^4 E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g)^2 = O(h^2 E^{\mathrm{GP}}_{2\mathrm{D}}(1,1,g)), \tag{3.29}$$

which tends to zero by assumption. Combining the bounds (3.11) and (3.28) finishes the proof.

□

3.3 Parameters of the GP Limit Theorem

By making use of scaled potentials in the GP functional we have seen that the GP energy satisfies a simple scaling relation (3.4). Hence, all calculations can be restricted to the case in which $N = 1$ and $L = 1$. For the numerical solution of the GP equation, which we present in Section 4.1, this means that the relevant input parameters are only the strength of the confining potential, represented by h, and the scattering length a for the interatomic forces.

However, the assumption $\bar{\rho}ah \to 0$ in **Theorem 4** involves the mean density. Then, for making the conclusions of the theorem accessible to a numerical analysis, we have to rewrite $\bar{\rho}$ in terms of a and h. To achieve this, we introduce a lengthscale λ and write, in d dimensions, $\bar{\rho} \sim 1/\lambda^d$. (Here N is set equal to 1, of course.) Now we go a step backward and make the substitutions $x = \lambda x'$ and $\phi(\mathbf{x}) = (1/\lambda^{d/2})\tilde{\phi}(\mathbf{x}')$ in the d-dimensional GP functional with coupling constant g. Then, if ϕ is normalized, so is $\tilde{\phi}$:

$$\|\tilde{\phi}(\mathbf{x}')\|^2_{L^2} = \int |\tilde{\phi}(\mathbf{x}/\lambda)|^2 \lambda^{-d} d^d\mathbf{x} = \int |\lambda^{d/2}\phi(\mathbf{x})|^2 \lambda^{-d} d^d\mathbf{x} = \|\phi(\mathbf{x})\|^2_{L^2} = 1 \tag{3.30}$$

If the confining potential is a homogeneous function of some degree s, i. e. $V(\lambda \mathbf{x}) = \lambda^s V(\mathbf{x})$, the contribution of its term in the energy functional is

$$\int V(\mathbf{x})|\phi(\mathbf{x})|^2 d^d\mathbf{x} = \lambda^s \int V(\mathbf{x}')|\tilde{\phi}(\mathbf{x}')|^2 d^d\mathbf{x}'. \tag{3.31}$$

On the other hand, for the interaction term we get

$$g\int |\phi(\mathbf{x})|^4 d^d\mathbf{x} = g\lambda^{-d} \int |\tilde{\phi}(\mathbf{x}')|^4 d^d\mathbf{x}' \tag{3.32}$$

and for the kinetic term

$$\int |\nabla\phi(\mathbf{x})|^2 d^d\mathbf{x} = \lambda^{-2} \int |\nabla'\tilde{\phi}(\mathbf{x}')|^2 d^d\mathbf{x}'. \tag{3.33}$$

Equating λ^s with $g\lambda^{-d}$ we obtain

$$\mathcal{E}^{\mathrm{GP}}_{\mathrm{3D}}[\phi] = g^{\frac{s}{s+d}} \left\{ g^{-\frac{s+2}{s+d}} \int |\nabla'\tilde{\phi}|^2 d^d\mathbf{x}' + \int V|\tilde{\phi}|^2 d^d\mathbf{x}' + \int |\tilde{\phi}|^4 d^d\mathbf{x}' \right\}. \tag{3.34}$$

For large g the kinetic term is small compared to the other terms ('Thomas-Fermi limit'). The extension of ϕ is $g^{1/(s+d)}$ times the extension of $\tilde{\phi}$ that is essentially independent of g. Thus the average density is

$$\bar{\rho} \sim g^{-\frac{d}{s+d}}. \tag{3.35}$$

For small g the average density is $O(1)$, so a formula valid for all g is

$$\bar{\rho} \sim (1+g)^{-\frac{d}{s+d}}. \tag{3.36}$$

In a two-dimensional harmonic trap, and with $g \sim a/h$, this specializes to

$$\bar{\rho} \sim \left(1+\frac{a}{h}\right)^{-1/2} = \left(\frac{a}{h}\right)^{-1/2} \left(1 + O\left(\frac{h}{a}\right)\right) \tag{3.37}$$

and $\bar{\rho} a h \sim a^{1/2} h^{3/2}(1 + O(h/a))$. Note also that

$$E^{\mathrm{GP}}_{\mathrm{2D}}(1,1,g) \sim \bar{\rho} a/h \sim \left(\frac{a}{h}\right)^{1/2} \left(1 + O\left(\frac{h}{a}\right)\right). \tag{3.38}$$

Furthermore, because of (3.8) and (3.29) the error term Δe in the limit theorem satisfies

$$\Delta e = O(a^{1/2} h^{3/2}) \left(1 + O\left(\frac{h}{a}\right)\right). \tag{3.39}$$

In Section 5 we shall compare the behaviour of Δe to the results obtained by numerical methods.

Chapter 4

Numerical Calculations

In this section we analyze the 3D $\rightarrow$ 2D limit of GP theory by means of numerical calculations. In order to achieve this, we have to solve the GP equation, which is the variational equation corresponding to the GP functional (see also Section 2.2.2). In three dimensions it reads

$$\left(-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + 4\pi a|\phi(\mathbf{x})|^2\right)\phi(\mathbf{x}) = \mu\phi(\mathbf{x}). \tag{4.1}$$

Here $\mu \equiv \mu^{\mathrm{GP}}$ is the chemical potential of the condensate. The wave function ϕ satisfies the normalization condition $\int |\phi|^2 = 1$. The first step in obtaining a solution to (4.1) is to rewrite the wave function using the Galerkin approximation, i. e. expanding ϕ in terms of a finite number of orthonormal basis functions [11]:

$$\phi(\mathbf{x}) = \sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z} c_{ijk}\chi_i(x)\chi_j(y)\chi_k(z) \tag{4.2}$$

The χ_n are chosen to be the eigenfunctions of the one-dimensional harmonic oscillator. N_x is the number of basis functions in x-direction used in the approximation. Let N be the total number of eigenfunctions in the expansion (4.2). Then we can introduce the short-hand notation

$$\phi(\mathbf{x}) = \sum_{i=0}^{N} C_i\Phi_i(\mathbf{x}). \tag{4.3}$$

By making this ansatz for the GP equation (4.1), multiplying it by another basis function $\Phi_j(\mathbf{x})$ and integrating, we get

$$\sum_i C_i \int \left[\Phi_j(\mathbf{x})\left(-\frac{1}{2}\nabla^2\Phi_i(\mathbf{x})\right) + V(\mathbf{x})\Phi_i(\mathbf{x})\Phi_j(\mathbf{x})\right] d^3x +$$
$$+ \sum_i C_i \int 4\pi a \sum_{k,l} C_k C_l \Phi_i(\mathbf{x})\Phi_j(\mathbf{x})\Phi_k(\mathbf{x})\Phi_l(\mathbf{x}) d^3x =$$
$$= \mu \sum_i C_i \int \Phi_i(\mathbf{x})\Phi_j(\mathbf{x}) d^3x. \tag{4.4}$$

Now, choosing V to be a harmonic potential, i. e. $V(\mathbf{x}) = (1/2)(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$, equation (4.4) becomes (note that $\int \Phi_i \Phi_j = \delta_{ij}$)

$$\sum_i C_i \left(E_i \delta_{ij} + 4\pi a \sum_{k,l} C_k C_l \int \Phi_i(\mathbf{x})\Phi_j(\mathbf{x})\Phi_k(\mathbf{x})\Phi_l(\mathbf{x}) d^3x \right) = \mu C_j \tag{4.5}$$

with E_i the energy of the 3D harmonic oscillator $E_i = (n_{xi} + 1/2)\omega_x + (n_{yi} + 1/2)\omega_y + (n_{zi} + 1/2)\omega_z$. Hence we have transformed the nonlinear differential equation (4.1) into a system of algebraic equations for the expansion coefficients C_i of the wave function and the eigenvalue μ:

$$\mathcal{A}\vec{C} = \mu\vec{C}. \tag{4.6}$$

The nonlinear term of $\mathcal{A}$ in (4.5) involves integrals of the form

$$J_{iklm} = \int \Phi_i \Phi_k \Phi_l \Phi_m d^3x, \tag{4.7}$$

where Φ is composed of well-known Hermite functions so that these integrals can be computed analytically [7]. The eigenvalue problem can then be solved by iteration, starting with the ground state of the harmonic oscillator or the Thomas-Fermi solution as an initial guess. In the context of Bose-Einstein condensation this method was first applied by Edwards and Burnett [10].

4.1 Numerical Solution of the Gross-Pitaevskii Equation

As already mentioned in Section 3.3, the relevant parameters determining the energy of a Bose-Einstein condensate in the Gross-Pitaevskii formalism are the scattering length a and the strength of the confining potential, given by h. In what follows we want to consider harmonic potentials that are homogeneous in the x- and y-directions, i. e. $\omega_x = \omega_y$, but strongly confining in z-direction with trap frequency $\omega_z = (\hbar/m)a_z^{-2} \equiv 1/h^2$ ($a_z \sim h$ is the oscillator length). Measuring energies in units of $\hbar\omega_x$, frequencies in units of ω_x and choosing a_x as the length unit, the 3D GP equation reads

ω_z	h	a	$E^{\mathrm{3D}}_{\mathrm{num}}$	μ_{num}	μ_{Bao}
4	0.5	15	6.43	8.37	8.37
4	0.5	1.5	3.78	4.36	4.36
4	0.5	0.15	3.11	3.22	-

Table 4.1: Parameters and results for the experimental setting of *Anderson et. al.* [1]. The chemical potential obtained is compared to values in literature [3].

$$\left(-\frac{1}{2}\nabla^2 + \frac{1}{2}\left(x^2+y^2+\omega_z^2 z^2\right) + 4\pi a|\phi(\mathbf{x})|^2\right)\phi(\mathbf{x}) = \mu\phi(\mathbf{x}). \tag{4.8}$$

We solve this equation making use of `Fortran`-routines written for this purpose [8, 33], especially in order to study the behavior of the energy if $h \to 0$ (i. e. $\omega_z \to \infty$). Table 4.1 lists results obtained by the programs for a sample solution of the 3D GP equation for typical parmeters a and ω_z. In fact, these values correspond to the experimental configuration studied by *Anderson et. al.* [1], leading to history's first observation of the Bose-condensed state. The wave function of the condensate is shown in Figure 4.1.

Remark. It should be noted that because of our normalization $\int |\phi|^2 = 1$ rather than $\int |\phi|^2 = N$ our parameter a corresponds physically to Na with N the particle number and a the scattering length of the interaction potential.

4.2 Solving the 2D GP Equation

In order to study dimensional reduction in terms of GP theory, we have to compare solutions of the 3D GP equation for increasing strength of the confining potentials to the corresponding 2D results.

Formally, the GP equation in two dimensions is obtained from (4.1) by considering a wave function

$$\phi(\mathbf{x}) = \varphi(x,y)s_h(z), \tag{4.9}$$

where s_h is the ground state of $(-\partial^2/\partial z^2 + \omega_z^2 z^2)/2$ with energy $\omega_z/2 = e^{\perp}/(2h^2)$ (this as well as the following statements shall be compared to Section 3.2). Multiplying the resulting equation by s_h and integrating over the z-coordinate yields

$$-\frac{1}{2}\nabla^2_{x,y}\varphi(x,y) + \frac{1}{2}(x+y)\,\varphi(x,y) + 4\pi a\int s_h(z)^4 dz|\varphi(x)|^2\varphi(x) = \left(\mu - \frac{\omega_z}{2}\right)\varphi(x). \tag{4.10}$$

Defining the coupling constant $g = (a/h)\int s^4 = a\int s_h^4$, we identify equation (4.10) as the variational equation of the 2D GP functional. The ground state

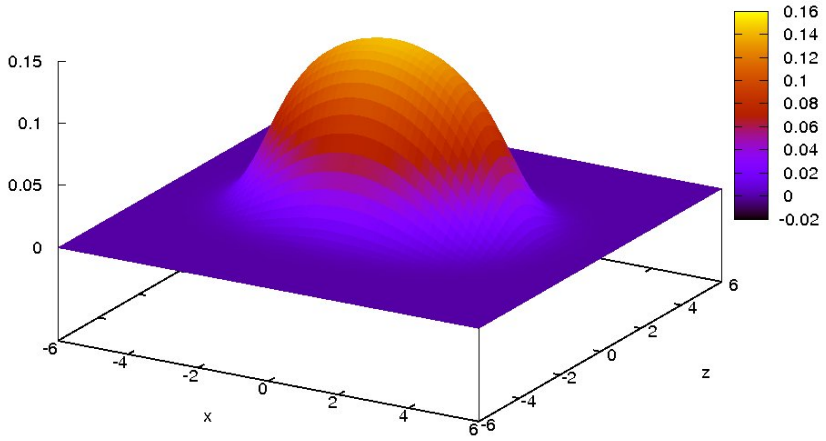

Figure 4.1: The figure shows the Gross-Pitaevskii ground state wave function ϕ_{GP} for a harmonic trap as studied experimentally by *Anderson et.al.* [1]. Here it was obtained by numerically solving the 3D GP equation for $a = 15$ and $h = 0.5$.

wave function s_h of the one-dimensional harmonic oscillator is of course well known:

$$s_h(z) = \frac{1}{\pi^{1/4} h^{1/2}} e^{-\frac{x^2}{2h^2}} = \left(\frac{\omega_z}{\pi}\right)^{1/4} e^{-\omega_z x^2/2} \tag{4.11}$$

Therefore, we can evaluate the coupling constant explicitly, and, introducing the chemical potential $\mu_{2\mathrm{D}}$, we get the 2D GP equation to be solved:

$$-\frac{1}{2}\nabla^2_{x,y}\varphi(x,y) + \frac{1}{2}(x+y)\varphi(x,y) + 2a\sqrt{2\pi\omega_z}\varphi(x,y) = \mu_{2\mathrm{D}}\varphi(x,y) \tag{4.12}$$

For a numerical study of this equation, I have modified the program code [33] to do 2D calculations (see Appendix for details). However, the following numerical results are based on the routines from [8].

Chapter 5

Results on the Convergence of E_{3D}^{GP} in the 2D Limit

The GP limit theorem in Section 3.2 shows that $E_{3D}^{GP} - e^{\perp}/h^2 \to E_{2D}^{GP}$ provided $h^2 E_{2D} \to 0$. The convergence is indeed linear in the parameter $h^2 E_{2D} \sim a^{1/2} h^{3/2}$ (see Section 3.3 for details). Can numerical calculations reflect this behaviour, moreover: can we explicitly compare error terms obtained analytically to results of numerical calculations?

5.1 Analytical vs. Numerical Approach

As seen from (3.5), the 2D GP energy is determined solely by the coupling constant g, i. e. by the ratio of a and h. Thus, fixing a/h means fixing $E_{2D}^{GP}(1, 1, g)$. In what follows we consider the two cases $a/h = 1$ and $a/h = 10$. Numerical solution of the 2D GP equation yields the energies (in units of $\hbar\omega_x$):

$$\begin{aligned} E_{2D}^{GP}\left(1, 1, \int s^4\right) &= 1.33427 \\ E_{2D}^{GP}\left(1, 1, 10\int s^4\right) &= 2.89934 \end{aligned}$$

Now let us turn to the 3D problem: increasing the strength of the confining potential (i. e. letting $h \to 0$) has to be done in a way such that a/h is still constant, as we wish to compare the resulting energies to the 2D values. The detailed data[1] we get, for both cases, is provided in Tables 5.1 and 5.2, where the potential is characterized by the oscillator length h and, equivalently, the trap frequency ω_z. Based on these results one can calculate Δe^{num}, which accounts

[1] There is nothing mysterious about the values 14.29 and 142.86. They originate from a certain choice of ω_z^{-1}, namely $\{\omega_z^{-1}\} = \{0.1, 0.07, 0.04, 0.02, 0.01, ...\}$.

ω_z	h	a	$E_{3D}^{num} - e^{\perp}/h^2$
10	0.3162	0.3162	1.33143
14.29	0.2646	0.2646	1.33226
25	0.2000	0.2000	1.33311
50	0.1414	0.1414	1.33369
100	0.1000	0.1000	1.33398
142.86	0.0837	0.0837	1.33407
250	0.0632	0.0632	1.33416
1000	0.0316	0.0316	1.33425

Table 5.1: Parameters and results for numerical calculations done with $a/h = 1$. The confinement is given by $h = \omega_z^{-1/2}$, where ω_z is measured in units of $\omega_x \equiv 1$.

ω_z	h	a	$E_{3D}^{num} - e^{\perp}/h^2$
25	0.2000	2.0000	2.87918
50	0.1414	1.4142	2.88915
100	0.1000	1.0000	2.89422
142.86	0.0837	0.8367	2.89575
250	0.0632	0.6325	2.89728
500	0.0447	0.4472	2.89831
1000	0.0316	0.3162	2.89882
1428.57	0.0265	0.2646	2.89898
2500	0.0200	0.2000	2.89913
5000	0.0141	0.1414	2.89925

Table 5.2: Parameters and results for numerical calculations done with $a/h = 10$.

for the error made when substituting the 3D GP energy by the 2D energy plus the confining energy, more precisely:

$$\Delta e^{\text{num}} = \left| 1 - \frac{E_{3D}^{\text{num}}(a,h) - e^{\perp}/h^2}{E_{2D}^{\text{num}}(g)} \right|. \tag{5.1}$$

On the other hand we have established analytical estimates. **Theorem 4** states that the error is bounded in the following way:

$$0 \leq 1 - \frac{E_{3D}^{\text{GP}}(a,h) - e^{\perp}/h^2}{E_{2D}^{\text{GP}}(g)} \leq \Delta e. \tag{5.2}$$

The form of Δe basically arises from Temple's inequality. In fact, using (3.18), (3.22) and (3.24) we derive from (3.27) the expression

$$\Delta e = \frac{\left(1 + 8\pi g \|\varphi_{\rm GP}\|_\infty^2/(e^\perp/h^2)\right)}{E_{\rm 2D}^{\rm GP}(g)} \cdot \frac{(8\pi)^2 \|\varphi_{\rm GP}\|_\infty^4 (a/h)^2 \left[\int s^6 - \left(\int s^4\right)^2\right]}{(\tilde{e}^\perp - e^\perp)/h^2 - 8\pi g \|\varphi_{\rm GP}\|_\infty^2}. \tag{5.3}$$

All the quantities in this formula (5.3) - listed in Table 5.3 - are known either from the numerical solution or can be computed without further ado. This allows us to compare - for every set of parameters a, h with $a/h = \text{const}$ - the values of Δe and $\Delta e^{\rm num}$. Tables 5.4 and 5.5 list the outcomes obtained and Figures 5.1 to 5.4 provide the corresponding graphics. The results of the numerical calculations are well embedded into the analytic bounds specified by 0 and Δe, as demanded by equation (5.2). In the plots they are represented by the abscissa and the crosses. For larger x-values, the linear plots show the slight dependence of Δe on higher order terms, while the logarithmic plots reveal equal characteristics of rigorous analysis and numerical solutions.

From (3.39) and (3.29) it is clear that for $h \to 0$ and $a/h = \text{const.}$ we have

$$\Delta e \sim h^2 E_{\rm 2D}^{\rm GP}(g) \sim a^{1/2} h^{3/2} \sim h^2. \tag{5.4}$$

This is in perfect agreement with the numerical data $\Delta e^{\rm num}$, where a detailed fit shows

$$\Delta e^{\rm num} \sim \left(a^{1/2} h^{3/2}\right)^{1.005}. \tag{5.5}$$

In order to compare our results to those reported in [2], we conclude from (5.2) and (3.38) that

$$\left|E_{\rm 3D}^{\rm GP}(a,h) - E_{\rm 2D}^{\rm GP}(g) - e^\perp/h^2\right| = E_{\rm 2D}^{\rm GP}(g)\Delta e \sim ah\left(1 + O\left(\frac{h}{a}\right)\right), \tag{5.6}$$

while [2] would give for this expression $ah|\ln h|$ (c. f. the equation on the top of p. 836 in [2]).

Both the analytical and numerical results thus show that the convergence is more rapid than stated in [2], where it is claimed (apparently based on numerical calculations) that $\Delta e^{\rm BGJMW} \sim (a \ln \omega_z)/\omega_z^{1/2}$. As a matter of fact, for $h \sim \omega_z^{-1/2}$ and $a\omega_z^{1/2} = \text{const.}$, we find

$$\Delta e^{\rm BGJMW} \sim \frac{\ln \omega_z}{\omega_z} > \frac{1}{\omega_z} \sim \Delta e \tag{5.7}$$

and thus faster convergence of the 3D GP energy.

a/h	E_{2D}^{GP}	$e^{\perp}/h^2$	$g = (a/h)\int s^4$	$\int s^6 - (\int s^4)^2$	$\|\varphi_{\mathrm{GP}}\|_\infty$
1	1.33427	ω_z	0.399	0.025	0.462
10	2.89937	ω_z	3.989	0.025	0.283

Table 5.3: Values needed to explicitly calculate the analytic error term given by formula (5.3).

ω_z	a	Δe^{num}	Δe
10	0.3162	2.13E-03	3.62E-02
14.29	0.2646	1.51E-03	2.32E-02
25	0.2000	8.70E-04	1.21E-02
50	0.1414	4.38E-04	5.68E-03
100	0.1000	2.19E-04	2.75E-03
142.86	0.0837	1.53E-04	1.91E-03
250	0.0632	8.42E-05	1.08E-03
500	0.0447	2.62E-05	5.36E-04
1000	0.0316	2.04E-05	2.67E-04

Table 5.4: Errors in the energy obtained by the numerical calculations Δe^{num} compared to the values Δe from the analytic bound. Calculations done with $a/h = 1$.

ω_z	a	Δe^{num}	Δe
25	2.0000	6.95E-03	2.10E-01
50	1.4142	3.51E-03	5.57E-02
100	1.0000	1.76E-03	2.17E-02
142.86	0.8367	1.24E-03	1.41E-02
250	0.6325	7.08E-04	7.53E-03
500	0.4472	3.54E-04	3.60E-03
1000	0.3162	1.77E-04	1.76E-03
1428.57	0.2646	1.24E-04	1.22E-03
2500	0.2000	6.95E-05	6.94E-04
5000	0.1414	3.06E-05	3.46E-04

Table 5.5: Errors in the energy obtained by the numerical calculations Δe^{num} compared to the values Δe from the analytic bound. Calculations done with $a/h = 10$.

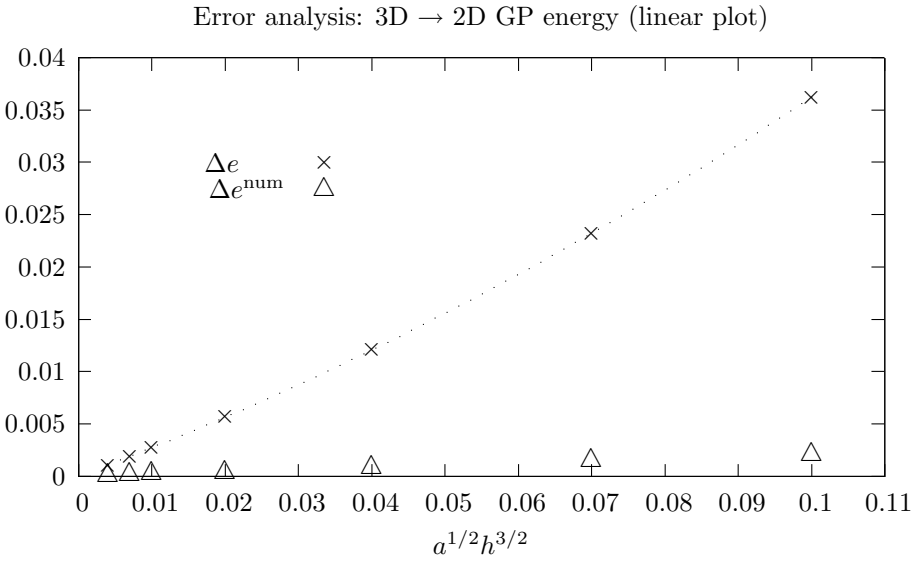

Figure 5.1: Comparison of numerical and analytical errors ($a/h = 1$). The triangles represent numerical results, whereas the crosses (resp. the dotted line) marks the analytic upper bound Δe (5.3).

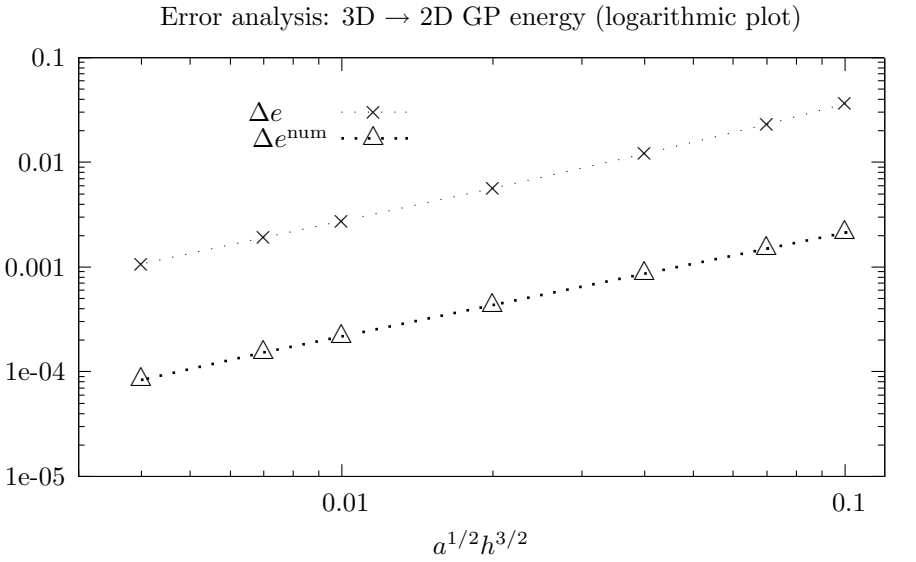

Figure 5.2: Comparison of numerical and analytical errors with logarithmic scales ($a/h = 1$). Both errors show the same dependence on the parameter $a^{1/2}h^{3/2}$. Numerically they differ by a factor of ~ 10.

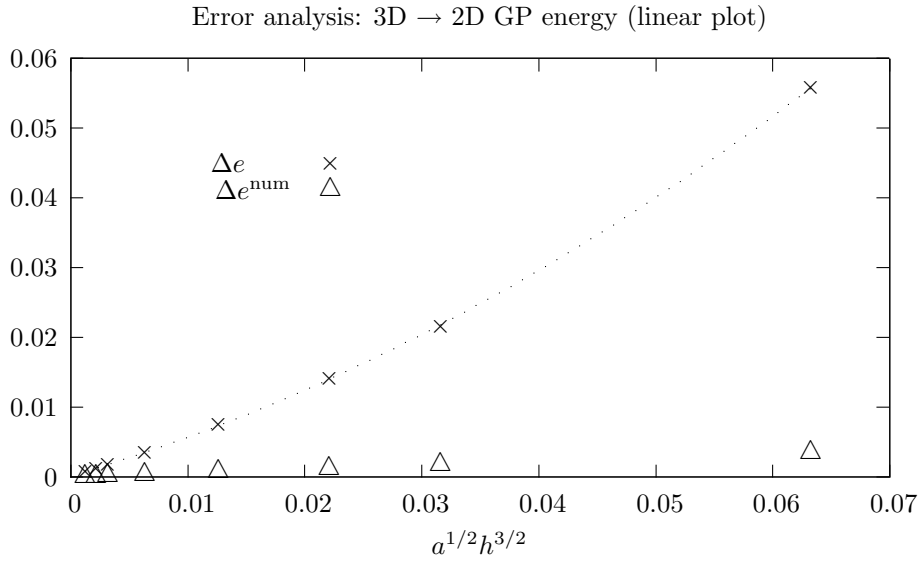

Figure 5.3: Comparison of numerical and analytical errors ($a/h = 10$). For large values of $a^{1/2}h^{3/2}$, the quadratic term in (5.3) becomes evident, whereas for $h \to 0$ only the leading order $\sim a^{1/2}h^{3/2}$ plays a significant role.

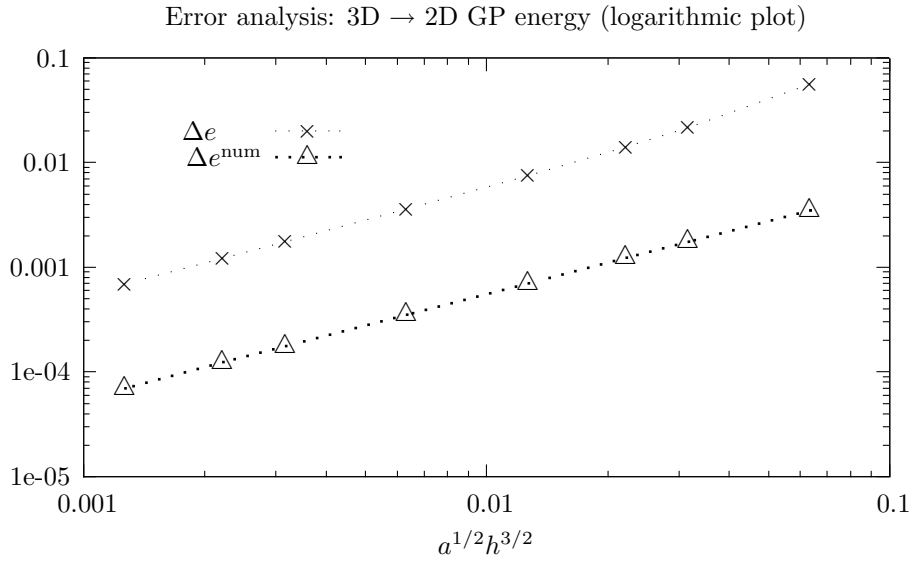

Figure 5.4: Comparison of numerical and analytical errors with logarithmic scales ($a/h = 10$).

5.2 Conclusions

We have studied dimensional reduction of Bose-Einstein condensates in terms of Gross-Pitaevskii theory. It was proved that for disc-shaped condensates the formula $E_{\mathrm{GP}}^{\mathrm{3D}} \approx E_{\mathrm{GP}}^{\mathrm{2D}} + e^{\perp}/h^2$ holds, where the error is of order $O(h^2 E_{\mathrm{GP}}^{\mathrm{2D}}) = O(a^{1/2}h^{3/2})$ and thus decreases with increasing confinement. This convergence of the energies obtained analytically was then compared to the results of numerical calculations on the Gross-Pitaevskii equations, yielding excellent agreement. Hence, the 3D GP energy can be well approximated by the two-dimensional quantity $E_{\mathrm{2D}}^{\mathrm{GP}}(N, L, g)$, plus the confining energy. These figures are of practical importance regarding numerical calculations, precisely because solving a two-dimensional problem rather than a 3D one means a significant reduction of computational time.

Appendix

Here we present excerpts from the source code written in the `Fortran 90` language and used for solving the 2D Gross-Pitaevskii equation. It is based on the 3D program reported in [33] and modified to apply to the two-dimensional problem.

Main Program

```
 PROGRAM oscl
  IMPLICIT NONE

  INTEGER :: i,j,m,s,ndim,r,istart,iham,ixmat,ixanh,ibuff,limit,no_terms,&
       nxmax,nymax,nzmax,n_max,ok,nmax,infile,nelec,idavid,nbas,&
       iparty,maxit,isteep,ithomas,imix,ientr,j_min,j_max,ndir
  INTEGER :: mx,my,mx_,my_,mz,mz_,icircle,i3dtype,icalc,nparticle,iplot
  real(kind=8) :: Wx,Wy,Wz,omega,alpha,scatlen,conv,delt,xmix,rmin,rmax,dr
  REAL(KIND=8),ALLOCATABLE,DIMENSION(:,:) :: inputpottwod
  !powers and coefficients specifying the perturbation potential
  integer, allocatable,dimension(:,:)::npower
  real(kind=8), allocatable,dimension(:)::coefpot
  !  REAL(KIND=8),ALLOCATABLE,DIMENSION(:,:) :: inputpotthreed
  !  REAL(KIND=8),ALLOCATABLE,DIMENSION(:) :: coef_pot
  REAL(KIND=8),ALLOCATABLE,DIMENSION(:,:,:) :: xstore,ystore,zstore
  integer,ALLOCATABLE::nx(:),ny(:),nz(:),idir(:,:)
  REAL(KIND=8),ALLOCATABLE,DIMENSION(:,:) :: ham
  REAL(KIND=8),allocatable,dimension(:,:) :: xmatrx,ymatrx,zmatrx
  character*80::line,potential
  logical::isotropic
!
  ndim=3
  infile=5
  ithomas=0
  ientr=0
  iplot=0
  read(*,*)line
  read(*,*)line
  line=adjustl(line)
  if(line(1:3)=='ISO')then
     !
```

```
   ! Case of isotropic (spherical) oscillator
   !
   i3dtype=1
   !
elseif(line(1:3)=='CYL')then
   !
   ! Case of cylindrical oscillator
   !
   i3dtype=2
   !
elseif(line(1:3)=='ANI')then
   !
   ! Case of anisotropic (oscillator)
   !
   i3dtype=3
   !
end if
!
if(i3dtype==1)then
   !
   read(*,*)line
   read(*,*)nmax
   nxmax=nmax
   nymax=nmax

   !
elseif(i3dtype==2)then
   !
   read(*,*)line
   read(*,*)nmax,nzmax
   nxmax=nmax
   nymax=nmax
   !
elseif(i3dtype==3)then
   !
   READ(*,*)line
   READ(*,*)nxmax,nymax,nzmax
   !
end if
!
n_max=(nxmax+1)*(nymax+1)
!
!
READ(*,*)line
read(*,*)no_terms
if(no_terms>0)then
   allocate(npower(ndim,no_terms),stat=ok)
   IF(ok /= 0) THEN
      WRITE(*,*)'ALLOCATION FAILURE FOR npower'
      STOP
   END IF
   !
```

```
      ALLOCATE(coefpot(no_terms),STAT=ok)
      IF(ok /= 0) THEN
         WRITE(*,*)'ALLOCATION FAILURE FOR COEFPOT'
         STOP
      END IF
      !
      read(*,*)line
      DO j=1,no_terms
         READ(*,*)coefpot(j),(npower(i,j),i=1,ndim)
      END DO
      write(*,*)' '
      !
      write(*,*)'Your perturbation potential is:'
      write(*,*)' '
      write(*,*)'Term #', '    Coeff', '    X Power', '   Y Power', '   Z Power'
      write(*,*)' '
      DO j=1,no_terms
         WRITE(*,33)j,coefpot(j),(npower(i,j),i=1,ndim)
      END DO
   end if
   write(*,*)' '
33 format(1x,i2.1,4x,f10.5,2x,i5.1,5x,i5.1,4x,i5.1)
   !
   !
   ! Read the frequencies
   !
   READ(*,*)line
   if(i3dtype==1)then
      !
      read(*,*)Wx,Wz
      wy=wx

      !
   elseif(i3dtype==2)then
      !
      read(*,*)wx,wz
      wy=wx
      !
   elseif(i3dtype==3)then
      !
      read(*,*)wx,wy,wz
      !
   end if
   !
   !
   ! read what type of calculation to do
   !
   ! icalc=1 => Gross-Pitaevskii calculation
   !      =2 => Hartree-Fock calculation
   !      =3 => Independent-Particle calculation
   !
   read(*,*)line
```

```
read(*,*)line
line=adjustl(line)
if(line(1:2)=='GP')then
   icalc=1
elseif(line(1:2)=='HF')then
   icalc=2
elseif(line(1:2)=='IN')then
   icalc=3
else
   write(*,*)'oscl: wrong choice of calculation type'
   write(*,*)'You gave calculation type=',line
   stop
end if
!
!
! Read the total no. of particles
!
read(*,*)line
read(*,*)nparticle
write(*,*)'Total No. of particles=',nparticle
!
! Read the scattering length (Harmonic Oscillator Units) for interacting
! particles
!
if(icalc==1.or.icalc==2)then
   read(*,*)line
   read(*,*)scatlen
end if
!
! Read the convergence threshold, maxit etc for SCF calculcalations
!
if(icalc==1.or.icalc==2)then
   read(*,*)line
   read(*,*)conv,maxit
end if
!
! Read whether parity is a good quantum number
!
iparty=0
read(*,*)line
read(*,*)line
line=adjustl(line)
if(line(1:3)=='PAR')iparty=1
if(iparty>0)then
  write(*,*)' '
  write(*,*)'Parity symmetry will be imposed on the wave function'
end if
!
!
! Read whether steepest descent procedure is desired or the normal SCF procedure
!
isteep=0
```

```
 delt=0.d0
 read(*,*,err=1)line
 read(*,*)line
 line=adjustl(line)
 if(line(1:5)=='STEEP')isteep=1
 !
 ! Read the time step needed for the steepest descent method
 !
 if(isteep>0)then
    write(*,*)' '
    write(*,*)'Steepest Descent Method chosen for Solving GP equation'
    read(*,*)line
    read(*,*)delt
    write(*,11)delt
11  format(1x,'Time step for Steepest-Descent Method:',3x,e7.2)
 else
    write(*,*)' '
    write(*,*)'Iterative diagonalization will be used to perform'
    write(*,*)'the SCF Calculations'
 end if
 !
 ! What starting orbitals to use (default is SHO ground state or from a file)
 !
 read(*,*)line
 read(*,*)line
 line=adjustl(line)
 if(line(1:6)=='THOMAS')ithomas=1
 if(ithomas>0)then
   write(*,*)' '
   write(*,*)'Thomas-Fermi solution will be used to start the calculations'
 else
   write(*,*)' '
   write(*,*)'SHO orbitals will be used to start the calculations'
 end if
 !
 ! Whether to user orbital mixin or not
 !
 imix=0
    write(*,*)' '
      read(*,*)line
      read(*,*)line
      line=adjustl(line)
      if(line(1:6)=='ORBMIX')then
         imix=1
      elseif(line(1:6)=='FOCKMI')then
         imix=2
      end if
      if(imix>0)then
        read(*,*)xmix
        if(imix==1)then
          write(*,*)'DURING SCF CYCLES, CONDENSATE MIXING WILL BE DONE'
          write(*,31)xmix
```

```
        elseif(imix==2)then
          write(*,*)'DURING SCF CYCLES, FOCK MATRIX MIXING WILL BE DONE'
          write(*,32)xmix
        end if
      end if
 31  format(' Starting fraction of new condensate in the total=',1f10.5)
 32  format(' Starting fraction of new Fock matrix in the total=',1f10.5)
  !
! See if condensate needs to be plotted
!
     read(*,*)line
     read(*,*)line
     line=adjustl(line)
     if(line(1:4)=='PLOT')iplot=1
     if(iplot>0)then
       read(*,*)rmin,rmax,dr
       read(*,*)ndir
       allocate(idir(3,ndir),stat=ok)
       if(ok/=0)then
         print*,'Program oscl: cannot allocate array idir'
         stop
       end if
       print*,' '
       print*,'Condensate will be plotted along directions'
       print*,' '
!
       do i=1,ndir
         read(*,*)(idir(j,i),j=1,3)
         print*,(idir(j,i),j=1,3)
       end do
!
     end if
     !See if Shannon entropy needs to be computed
     !
     read(*,*)line
     read(*,*)line
     line=adjustl(line)
     if(line(1:3)=='ENT')ientr=1
     j_min=0
     j_max=0
     read(*,*,err=1)j_min,j_max
1 continue
  !
  if(no_terms>0)then
     !
     allocate(xmatrx(0:nxmax,0:nxmax),stat=ok)
     if (ok /= 0)then
        write(*,*)'xmatrx allocation failure'
        stop
     end if
     !
     allocate(ymatrx(0:nymax,0:nymax),stat=ok)
```

```
   if (ok /= 0)then
      write(*,*)'ymatrx allocation failure'
      stop
   end if
   !
   allocate(zmatrx(0:nzmax,0:nzmax),stat=ok)
   if (ok /= 0)then
      write(*,*)'zmatrx allocation failure'
      stop
   end if
   !
   call xmat_0(xmatrx,nxmax)
   call xmat_0(ymatrx,nymax)
   call xmat_0(zmatrx,nzmax)
   do i=0,nymax
      do j=0,nymax
         ymatrx(i,j)=ymatrx(i,j)/sqrt(wy/wx)
      end do
   end do
   !
   do i=0,nzmax
      do j=0,nzmax
         zmatrx(i,j)=zmatrx(i,j)/sqrt(wz/wx)
      end do
   end do
end if
!
!
if(i3dtype==1)then
   call basgen3d_iso(nmax,nx,ny,nbas,iparty,1)
elseif(i3dtype==2)then
   call basgen3d_cyl(nmax,nzmax,nx,ny,nz,Wx,Wz,nbas,iparty,1)
elseif(i3dtype==3)then
   call basgen3d_aniso(nxmax,nymax,nzmax,nx,ny,nz,Wx,Wy,Wz,nbas,iparty,1)
end if
ALLOCATE(nx(nbas),STAT=ok)
IF (ok /= 0) THEN
   WRITE(*,*)'ALLOCATION FAILURE FOR nx'
   STOP
END IF

ALLOCATE(ny(nbas),STAT=ok)
IF (ok /= 0) THEN
   WRITE(*,*)'ALLOCATION FAILURE FOR ny'
   STOP
END IF

! ALLOCATE(nz(nbas),STAT=ok)
! IF (ok /= 0) THEN
!    WRITE(*,*)'ALLOCATION FAILURE FOR nz'
!    STOP
! END IF
```

```
  nx=0
  ny=0
  ! nz=0
  !
  if(i3dtype==1)then
     call basgen3d_iso(nmax,nx,ny,nbas,iparty,2)
  elseif(i3dtype==2)then
     call basgen3d_cyl(nmax,nzmax,nx,ny,nz,Wx,Wz,nbas,iparty,2)
  elseif(i3dtype==3)then
     call basgen3d_aniso(nxmax,nymax,nzmax,nx,ny,nz,Wx,Wy,Wz,nbas,iparty,2)
  end if
  !
  ALLOCATE(ham(nbas,nbas),STAT=ok)
  IF (ok /= 0) THEN
     WRITE(*,*)'ALLOCATION FAILURE FOR HAM'
     STOP
  END IF
  !
  ham=0.d0
  !
  !
  call ham0_3d(wy/wx,wz/wx,ham,xmatrx,ymatrx,zmatrx,npower,&
       coefpot,nx,ny,nbas,no_terms,nxmax,nymax)
  !
  if((icalc==1.or.icalc==2))then
     call bec_drv(ham,nbas,ndim,nx,ny,Wx,Wy,Wz,nxmax,nymax,&
          scatlen,nparticle,conv,icalc,maxit,isteep,ithomas,&
          delt,ientr,j_min,j_max,imix,xmix)
  end if
!
  if(iplot>0)call cond_plot(nxmax,nymax,nx,ny,ham,wx,wy,wz,nbas,ndir,&
                            idir,rmin,rmax,dr)
!
!write(*,*)'byeeeee'



END PROGRAM oscl
```

Subroutines

For the subroutines, analogous substitutions as reported here for the main program have to be performed on the routines from [33].

Bibliography

[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wiemann, and E. A. Cornell. Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor. *Science*, 269:198–201, (1995).

[2] W. Bao, Y. Ge, D. Jaksch, P. A. Markovich, and R. M. Weishäupl. Convergence rate of dimension reduction in Bose-Einstein condensates. *Comp. Phys. Comm.*, 177:832–850, (2007).

[3] W. Bao and W. Tang. Ground-state Solution of Bose-Einstein Condensate by Directly Minimizing the Energy Functional. *J. Comput. Phys.*, 187:230–254, (2003).

[4] G. Baym and C. J. Pethick. Ground-State Properties of Magnetically Trapped Bose-Condensed Rubidium Gas . *Phys. Rev. Lett.*, 76:6–9, (1996).

[5] N. N. Bogoliubov. On the Theory of Superfluidity. *J. Phys. (USSR)*, 11:23, (1947).

[6] S. N. Bose. Plancks Gesetz und Lichtquantenhypothese. *Z. Physik*, 26:178–181, (1924).

[7] I. W. Busbridge. Some Integrals Involving Hermite Polynomials. *J. London Math. Soc.*, 23:133–141, (1948).

[8] C. M. Dion and E. Cancès. Ground State of the Time-independent Gross-Pitaevskii Equation. *Comput. Phys. Comm.*, 177:787–798, (2007).

[9] F. J. Dyson. Ground-State Energy of a Hard-Sphere Gas. *Phys. Rev.*, 106:20–26, (1957).

[10] M. Edwards and K. Burnett. Numerical Solution of the Nonlinear Schrödinger Equation for Small Samples of Trapped Neutral Atoms. *Phys. Rev.*, A 51:1382, (1995).

[11] M. Edwards, R. J. Dodd, C. W. Clark, P. A. Ruprecht, and K. Burnett. Properties of a Bose-Einstein Condensate in an Anisotropic Harmonic Potential. *Phys. Rev.*, A 53:1950–1953, (1996).

[12] A. Einstein. Quantentheorie des einatomigen idealen Gases. *Sitzber. Kgl. Preuss. Akad. Wiss.*, pages 3–14, (1925).

[13] A. Görlitz et. al. Realization of Bose-Einstein Condensates in Lower Dimension. *Phys. Rev. Lett.*, 87:1–4, (2001).

[14] M. Greiner, I. Bloch, O. Mandel, T. W. Hänsch, and T. Esslinger. Exploring Phase Coherence in a 2D Lattice of Bose-Einstein Condensates. *Phys. Rev. Lett.*, 87:160405, (2001).

[15] E. P. Gross. Structure of a Quantized Vortex in Boson Systems. *Nuovo Cimento*, 20:454–466, (1961).

[16] T. Kinoshita, T. Wenger, and D. S. Weiss. Observation of a One-Dimensional Tonks-Girardeau Gas. *Science*, 305:1125, (2004).

[17] W. Lenz. Die Wellenfunktion und Geschwindigkeitsverteilung des entarteten Gases. *Z. Phys.*, 56:778–789, (1929).

[18] E. H. Lieb and W. Liniger. Exact Analysis of an Interacting Bose Gas. I. The General Solution and the Ground State . *Phys. Rev.*, 130:1605–1616, (1963).

[19] E. H. Lieb and R. Seiringer. Proof of Bose-Einstein Condensation for Dilute Trapped Gases. *Phys. Rev. Lett.*, 88:170409–1–4, (2002).

[20] E. H. Lieb, R. Seiringer, J.P. Solovej, and J. Yngvason. The Mathematics of the Bose gas and its Condensation. *Birkhäuser, Basel*, (2005).

[21] E. H. Lieb, R. Seiringer, and J. Yngvason. Bosons in a Trap: A Rigorous Derivation of the Gross-Pitaevskii Energy Functional. *Phys. Rev.*, A 61(043602), (2000).

[22] E. H. Lieb, R. Seiringer, and J. Yngvason. A Rigorous Derivation of the Gross-Pitaevskii Energy Functional for a Two-dimensional Bose Gas. *Comm. Math. Phys.*, 224:17, (2001).

[23] E. H. Lieb and J. Yngvason. Ground State Energy of the low density Bose Gas. *Phys. Rev. Lett.*, 80:2504–2507, (1998).

[24] E. H. Lieb and J. Yngvason. The Ground State Energy of a Dilute Two-dimensional Bose Gas. *J. Stat. Phys.*, 103:509, (2001).

[25] F. London. On the Bose-Einstein Condensation. *Phys. Rev.*, 54:947 – 954, (1938).

[26] O. Penrose and L. Onsager. Bose-Einstein Condensation of Dilute Gases. *Phys. Rev.*, 104:576–84, (1956).

[27] L. P. Pitaevskii. Vortex lines in an imperfect Bose gas. *Sov. Phys. JETP.*, 13:451–454, (1961).

[28] M. Schick. Two-Dimensional System of Hard Core Bosons. *Phys. Rev. A*, 3:1067–1073, (1971).

[29] K. Schnee and J. Yngvason. Bosons in Disc-Shaped Traps: From 3D to 2D. *Comm. Math. Phys.*, 269:659–691, (2007).

[30] R. Seiringer. Diploma Thesis. *University of Vienna*, (1999).

[31] R. Seiringer. Dilute, Trapped Bose Gases and Bose-Einstein Condensation. In J. Derezinski and H. Siedentop, editors, *Large Coulomb Systems, Lect. Notes Phys.*, volume 695, pages 251–276. Springer, (2006).

[32] G. Temple. The Theory of Rayleigh's Principle as applied to Continuous Systems. *Proc. Roy. Soc. London*, A 119:276–293, (1928).

[33] R. P. Tiwari and A. Shukla. A Basis-set based Fortran Program to solve the Gross-Pitaevskii Equation for Dilute Bose gases in Harmonic and Anharmonic Traps. *Comput. Phys. Comm.*, 174:966–982, (2006).

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