Rigorous Approach to Bose-Einstein Condensation

Marin Bukov

Bachelor Thesis
Mathematics Department
LMU Munich

Advisor: Prof. László Erdős, Ph.D.

July 24, 2011

Declaration of Authorship

I declare that this thesis was composed by myself and that the work contained therein is my own, except where explicitly stated otherwise in the text.

Marin Bukov
July 24, 2011

Acknowledgements

I would very much like to express my gratitude for being able to do my bachelor thesis project in the chair of Prof. László Erdős, Ph.D. I am extremely thankful both to him and Alessandro Michelangeli, Ph.D. for the support and the patience they had with me in the process of understanding the core ideas behind the main topic. Special thanks go to Alessandro for always finding time to help me in the constant struggle with the numerous technical and conceptual issues, be it related or unrelated to the topic, and to László for being such a good lecturer. I would also like to thank Tim Tom (although he didn't want me to put his name over here) and to Mario for proof-reading some of my calculations, as well as to Jonas for the thesis template and the moral support!

Contents

Chapter 1

Introduction

1.1 General Motivation

According to the current state of our knowlegde, ordinary matter is believed to be composed of particles interacting on scales $\sim 10^{-10}m$. It is a well-established fact that these particles obey the laws of Quantum Mechanics and can be divided into two categories - bosons and fermions. This distinction has turned out to be necessary, since their distribution in a system of macroscopic size obeys different quantum statistics. Identical fermions cannot occupy the same quantum states, whereas identical bosons can. The two species of particles differ in a fundamental feature, the spin. While fermions have half-integer spin, boson have integer spin. Not surprisingly, the different nature of these particles gives rise to a multitude of interesting physical phenomena.

One of them is the Bose-Einstein condensation. It is defined as a *macroscopic occupation of a single particle state*. This remarkable phenomenon involves bosons only. Bose gases can be roughly divided into two categories, with respect to their mathematical description. The first one is the non-interacting gas: particles move freely, i.e. without experiencing any force due to the presence of the other ones or some external source. This is the simplest approximation and can, therefore, be described mathematically without many complications as will be shown in a subsequent section. The fact that it can be solved completely makes it a starting point for the general discussion of the highly non-trivial interacting gas model.

Interactions can occur in different ways. It can be distinguished between inter-particle interactions and interactions of the particles with an external potential. A physically fundamental interaction is the Coloumb interaction which is responsible for the attraction and repulsion of charged particles. Another important example is an external field, typically a magnetic or electric one. Such fields shift and split the energy levels the bosons occupy. In general, the presence of interactions imposes great complications on the solvability of the mathematical equations.

However, under certain assumptions, one can still rigorously explain the occurrence of Bose-Einstein condensation in weakly interacting, dilute systems. This shall be formalised mathematically with a suitable scaling limit that produces interactions that are very strong on a very short distances. The most natural assumption of them all is to consider only two-body interactions, representing the simplest possible case in a system of many particles. Another typical simplification is to neglect energy fluctuations due to finite temperature, effectively considering zero-temperature gases. One reason for this is that the occurrence of the particle condensate is usually observed at temperatures much smaller than one Kelvin. The verification of such a theory should not present difficulties, since condensates are already realised experimentally.

Very often the simplifications, considered in the previous paragraph, are not enough to make rigorous statements. The limit considered in the following also assumes that the gas is sufficiently dilute, imposing a constraint on its density. Every interaction can be effectively described by a limited number of parameters. Under strong dilution, it turns out that the only effective parameter entering the theory is the so-called ‘s-wave scattering length’ which, roughly speaking, encodes the effective range of the interaction as well as its strength. Conversely, for a given specific potential, the value of a can also be calculated. From an experimental point of view it is much easier to measure the effective length scale of the interactions between particles than the concrete functional dependence of the potential. In the following, the term *dilute* shall suggest that the average distance between any two particles is much larger than the scattering length. Further assumptions, whenever important, shall be discussed in subsequent chapters.

In this thesis the following topics shall be discussed:

- BEC from historical point of view: development of the main theoretical ideas and their confirmation through experiment.
- Foundations of Quantum Mechanics - preliminaries and postulates.
- Analysis of the free Bose gas and its condensation. Several peculiar properties are derived.
- The weakly interacting dilute Bose gas: rigorous upper and lower bounds to the ground state energy in the dilute limit are derived.
- The Gross-Pitaevskii theory - BEC of weakly interacting particles in a trap: upper and lower bounds to the ground state energy in the Gross-Pitaevskii limit.

1.2 Historical Development of Theory and Experiment

The subject of Bose-Einstein condensation first entered the scene of theoretical physics in 1924 when Einstein predicted a phase transition in the most popular spin-one particle system known at that time - photons. His paper was based on previous ideas by Bose on the statistics of light quanta. The phenomenon appeared naturally as a consequence of quantum statistical effects and represented a modification of concepts by Bose about the photon energy occupation distribution with no fixed total particle number. Einstein translated the paper himself from English to German and eventually submitted it for publication to leading German science journals [4]. He also extended and generalised Bose's notions to fixed particle number - a feature thought improper of systems of photons until very recently due to absorption by the walls of the container the photons are put in.

While the phenomenon revealed the power of quantum statistics in its full beauty, its predictions remained of no practical importance for quite a long time, and have therefore been treated rather as a 'theoretical or mathematical curiosity'. In 1938, first experimental significance appeared when London tried to explain superfluidity in liquid He in terms of Bose-Einstein condensation [19]. Meanwhile, the first quantum theory of hydrodynamics by Landau appeared to take different approach to the subject, confronting London's ideas. Few years later, in 1941 Landau succeeded in publishing the first self-consistent theory of superfluidity explaining the phenomenon as a spectrum of elementary excitations.

Strange as it may seem, it took science more than 25 years to develop trustful predictions about interacting Bose gases and their condensation. This came true in 1947 when the first microscopic theory was published by Bogoliubov [1]. While being intuitively correct, it has later been found to contain some major gaps and flaws. Subsequently, by 1950, the inconsistencies were removed due to the work of Landau and Lifschitz [10], Onsager and Penrose [23, 24], who proposed a physical theory explaining the weakly interacting gas case. However, it lacked a rigorous mathematical treatment.

In the meanwhile, experimental studies had confirmed Landau's theory by attempting to measure BEC indirectly via its momentum distribution, representing the most reliable method for the time. Noteworthy are also the predictions of quantum vortices in superfluids by Onsager (1949) [22] and Feynman (1955) [5], for they appeared to be in perfect agreement with the experiments due to Hall and Vinen from 1956.

The major breakthrough in confirming the already well-stablished theory came along with the investigation of liquid He which happened to be the first observed BEC. However, the relatively strong interactions between its molecules lead to a reduction of the ground state occupancy, providing a significant challenge on the direct observation of the condensate. Therefore, scientists looked for weakly interacting Bose gases to maximise the fraction of particles in the lowest energy state, also known as the ground state. The major difficulty thereby appeared to be the low temperature limit, in which increased intermolecular forces bind the gas molecules together to form liquids or even solids, violating the assumptions of a dilute limit.

The experimental studies on dilute Bose gases date to the 1970s when various laser techniques, such as magnetic and optical trapping, have been developed. The cooling procedure was performed in basically three steps: first, the gas is put in a dilution refrigerator to lower the temperature of its molecules. This was succeeded by trapping it in an external magnetic field aligning the probe spins. Evaporative cooling was finally used to lower the gas temperature even further. In the 1980s the major breakthrough in laser technology allowed for refinement and improvement of the techniques mentioned above merging the last two steps in to a single one, called magneto-optical cooling. These experiments revealed the hidden condensation potential of alkali atoms and their cooling-favouring structure. These were expected to have well-defined and relatively easy to access optical transitions due to the 1s orbital being single occupied which, combined with the transition rules dictated by conservation of angular momentum, opened the door to controlling the internal energy of the system. Hence, its temperature was achieved to be reduced to several Kelvins.

This successful trend was continued throughout the 1990s when the research groups led by Ketterle, Boulder, Wieman and Cornell finally reached the critical temperature and density necessary for BEC to be observed. The first condensates consisted of ^{87}Rb, ^{23}Na, ^{7}Li, succeeded by spin-polarised H, metastable ^{4}He, ^{41}K atoms, and many others. The successful cooling procedure turned out to use laser cooling as a pre-cooling only. This already achieves ultralow temperatures. The gas is then confined in a magneto-optical trap. Evaporative cooling is used last as a final ingredient to decrease the temperature below the critical one ultimately enabling a condensation. This major success culminated in the 2001 Nobel Prize in physics going to Cornell, Ketterle and Wieman 'for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates' [9].

To summarise briefly, BEC turned out to have application to various fields of physics and many different physical systems. Among the most important of them is the theory of superconductivity which is basically understood as a BEC of pairs of electron, called Cooper pairs and reveals certain similarities to superfluidity. Pairs of fermions are also thought to condense under specific circumstances in atomic nuclei where one finds proton-proton, neutron-neutron and proton-neutron pairs. Last but not least, recent research has shown various applications to stellar physics, astronomy and particle physics [21].

1.3 Quantum Mechanics Preliminaries

Quantum Mechanics is a theory of physics built upon several assumptions, called postulates. These have been empirically verified and widely accepted as true. In this section we present the postulates and discuss the most important examples with respect to the subsequent discussion on Bose-Einstein condensation. In the following, the Schrödinger picture will be adopted[1].

1.3.1 One-Body Quantum Mechanics

Postulate 1.1 (Postulate I)**.** *The physical state of a 3-dimensional quantum mechanical system at any given time t is completely described by a normalised* ***state vector*** *ψ_t in the separable Hilbert space $L^2(\mathbb{R}^3, \mathrm{d}x)$.*

Postulate 1.2 (Postulate II)**.** *Every physically measurable property of the system is associated with a self-adjoint operator $\hat{O}$, called* ***observable****.*

The most important operator is the Hamiltonian $\hat{H}$ and is given by:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}_t(x) \tag{1.1}$$

[1] for the conceptually different Heisenberg picture, the reader is referred to the literature.

where $\hat{V}_t(x)$ is the time-dependent potential the particle is confined in and $\hbar = 1.064 \times 10^{-34} Js$ is the reduced Planck constant. Mathematically $\hat{V}_t$ is defined as a multiplication operator. Throughout this thesis, $\hat{V}$ and hence $\hat{H}$ will be taken to be time-independent.

Postulate 1.3 (Postulate III)**.** *A measurement of a physical property associated with an operator $\hat{O}$ in the state ψ always reproduces the expectation $\langle \psi, \hat{O}\psi \rangle$. If additionally ψ is an eigenvector of $\hat{O}$, a measurement gives the eigenvalues of $\hat{O}$, since ψ is assumed to be normalised.*

By the Spectral Theorem, all self-adjoint operators are uniquely determined by their spectrum. The points belonging to the point spectrum are called eigenvalues and the corresponding eigenvectors - **eigenstates**.

Postulate 1.4 (Postulate IV)**.** *Measuring a property, described by the operator $\hat{O}$, in the state ψ will give with probability*

$$p_n = \frac{\langle \psi | \hat{P}_n \psi \rangle}{\langle \psi, \psi \rangle} \tag{1.2}$$

the value λ_n. Here $\hat{P}_n$ is the projector operator onto the eigenspace determined by the eigenvalue λ_n of $\hat{O}$.

Postulate 1.5 (Postulate V: Wave Function Collapse)**.** *Whenever a measurement of a physical property in the state ψ gives the value λ_n the system is found after the measuring in the state*

$$\psi_n = \frac{\hat{P}_n \psi}{\sqrt{\langle \psi | \hat{P}_n \psi \rangle}}. \tag{1.3}$$

This is mathematically equivalent to a normalised projection onto the subspace corresponding to λ_n.

Postulate 1.6 (Postulate VI: Schrödinger's Equation)**.** *The time evolution of a state ψ_t is given by the time-dependent Schrödinger equation:*

$$\hat{H}\psi_t(x) = i\hbar \partial_t \psi_t(x) \tag{1.4}$$

with the ***Hamiltonian*** *(or the total energy operator) $\hat{H}$.*

Whenever $\hat{H}$ does not depend on t and when we are interested in stationary solutions to (1.4), i.e. assuming a trivial time dependence $\psi_t(x) = \psi(x)e^{-iEt/\hbar}$, we end up with the time-independent Schrödinger equation:

$$\hat{H}\psi(x) = E\psi(x), \tag{1.5}$$

and its solutions are called stationary states.

Postulate 1.7 (Postulate VII: Correspondence Principle)**.** *Any observable in classical mechanics corresponds to an operator in quantum mechanics by replacing x and p via the operators $\hat{x}$ and $\hat{p}$. If necessary, the observable must be symmetrised. The position and momentum operators $\hat{x}$ and $\hat{p} = -i\hbar\nabla$ satisfy the canonical commutator relations*

$$\begin{aligned} [\hat{x}_j, \hat{p}_k] &= i\hbar\delta_{jk} \\ [\hat{x}_j, \hat{x}_k] &= [\hat{p}_j, \hat{p}_k] = 0. \end{aligned} \tag{1.6}$$

The above postulates describe the quantum mechanics of a single particle. In order to understand collective phenomena, such as Bose-Einstein condensation, some of the above statements have to be modified to the many-body case.

1.3.2 Many-Body Quantum Mechanics

In many-body quantum mechanics one usually considers a system of N particles in three-dimensional space. In particular the postulates are slightly modified through the introduction of a density operator $\hat{\rho}$ that generalises the wave-function concept[2].

Postulate 1.8 (Postulate I'). *The physical state of a 3-dimensional quantum mechanical system is completely described by a positive, normalised self-adjoint trace-class operator $\hat{\rho}$, $tr\hat{\rho} = N$, on the Hilbert space $L^2(\mathbb{R}^{3N})$, called* ***density operator*** *or* ***density matrix****.*

This definition allows us to distinguish between to types of states. *Pure states* are defined as projections onto the subspace spanned by a single state, whose wave function is given by a vector $\psi \in L^2(\mathbb{R}^{3N})$. Additionally, a many-body system may consist of particles in different states. In this latter case, the system is called to be in a *mixed state*, and $\hat{\rho}$ does not represent a projection any more. Since every compact self-adjoint operator has a well-defined spectral decomposition, the eigenvalues of ρ are naturally interpreted as occupation numbers of particles in the system.

Postulate 1.9 (Postulate IV'). *The expectation value of the operator $\hat{O}$, in the state $\hat{\rho}$ is given by*

$$\langle \hat{O} \rangle = tr(\hat{\rho}\hat{O}). \tag{1.7}$$

Postulate 1.10 (Postulate VI'). *The time evolution of the density operator is governed by the von Neumann equation:*

$$i\hbar\partial_t\hat{\rho}(t) = [\hat{H}(t), \hat{\rho}(t)]. \tag{1.8}$$

An N-particle system can be described also by a wave function Ψ in the tensor product space $L^2(\mathbb{R}^{3N})$. A priori, there is no restriction on its symmetry. However, it has been experimentally verified that many-body wave functions, describing a collection of fermions or bosons only, have well-defined symmetry.

Postulate 1.11 (Pauli Exclusion Principle). *The joint wave function of a collection of N bosons is always symmetric under exchange of any two particles. For N fermions it is always antisymmetric, i.e.*

$$\begin{aligned} \Psi_B(x_1, ..., y, ..., z, ...x_N) &= \Psi_B(x_1, ..., z, ..., y, ...x_N) \\ \Psi_F(x_1, ..., y, ..., z, ...x_N) &= -\Psi_F(x_1, ..., z, ..., y, ...x_N). \end{aligned} \tag{1.9}$$

This fact allows us to restrict our attention only to the subspace of the symmetric and anti-symmetric states. Given N arbitrary one-particle wave functions $f_1, ..., f_N$, one can construct a bosonic or fermionic state as:

$$\begin{aligned} \Psi_F(x_1, ..., x_N) &= (f_1 \wedge ... \wedge f_N)(x_1, ..., x_N) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (-1)^\pi \prod_{j=1}^{N} f_j(x_{\psi(j)}) \\ \Psi_B(x_1, ..., x_N) &= \frac{1}{N!} \sum_{\pi \in S_N} \prod_{j=1}^{N} f_j(x_{\psi(j)}) \end{aligned} \tag{1.10}$$

The symmetry properties make these functions easy to handle in complex calculations.

[2] density operators also exist in the one-body case and are given by projections $\hat{\rho} = |\psi\rangle\langle\psi|$.

1.4 Analysis of the Free Bose Gas

When describing a large system of N particles, one is often not interested in the behaviour of the single particles themselves, but in the properties of the system as a whole. The main concept of thermodynamics is that only a handful of variables, called state variables, are enough for the full description of a macroscopic system in equilibrium. What connects the micro to the macrostates is an insight by Boltzmann: since there are very many ways the particles can be arranged, the macroscopic state would consist of the most probable microscopic ones that maximise the entropy of the system. According to quantum statistical mechanics, one defines a density operator to a system via its Hamiltonian. In the following, we only need the grand canonical ensemble, where one considers a system of fixed volume V and chemical potential μ, connected to a larger system called reservoir. Among its main features are the exchange of energy and particles with the reservoir. We proceed, following [7], by defining the grand canonical **partition function** as

$$Z_{gc} = \mathrm{tr}(e^{-\beta(\hat{H}-\mu\hat{N})}) = \sum_{n=1}^{\infty}\langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle = \sum_{n=1}^{\infty} e^{-\beta(E_n-\mu n)} \tag{1.11}$$

where $\hat{H}$ is the Hamiltonian with energies E_n, $\mu < 0$ - the chemical potential, i.e. the amount of energy needed to take a particle out of the system (and back to the reservoir), and $\hat{N}$ the particle number operator, satisfying $\hat{N}|n\rangle = n|n\rangle$. The parameter $\beta = 1/k_BT$ has units of inverse temperature, with $k_B = 1.380JK^{-1}$ being the Boltzmann constant. The partition function is used as a normalisation constant to the density operator of the system, which represents a mixed state and is given by

$$\hat{\rho} = \frac{1}{Z_{gc}} e^{-\beta(\hat{H}-\mu\hat{N})}. \tag{1.12}$$

To calculate the expectation value of an observable $\hat{O}$ in the state corresponding to the density $\hat{\rho}$, one has to compute

$$\langle\hat{O}\rangle = \mathrm{tr}(\hat{O}\hat{\rho}). \tag{1.13}$$

This definition incorporates both the quantum mechanical and the statistical expectations.

The relation between micro and macro physics is given by the grand canonical potential Ω as

$$\Omega = -\beta\log(Z_{gc}). \tag{1.14}$$

This is the starting point for deriving the thermodynamics of the system, since quantities, such as the expectation values of particle number N, entropy S, energy E, pressure p, and volume V are related to the grand potential via the equations of state.

Very often, one considers a system in a finite box of side length L and particle number N since this problem yields a discrete spectrum for the Hamiltonian and the calculations become simpler. The *thermodynamic limit* is then defined as letting $N \to \infty$ and $L \to \infty$ while keeping the density $\rho = N/L^3$ fixed. In the following we shall apply Quantum Statistical Mechanics to a non-interacting gas of bosons.

We begin by computing the grand partition function. Consider a system of N free bosons with energies E_i and degeneracies n_i, respectively, at a given chemical potential μ. Clearly, the total number of particles is given by $N = \sum_i n_i$ and the total energy by $E = \sum_i E_i n_i$. The grand canonical partition function then amounts to:

$$\begin{aligned} Z_{gc} &= \mathrm{tr}(e^{-\beta(\hat{H}-\mu\hat{N})}) = \sum_{\{n_i\}} \exp\Big(-\beta(\sum_{i=1}^{N} n_i E_i - \mu \sum_{i=1}^{N} n_i)\Big) \\ &= \sum_{\{n_i\}} \exp\Big(-\beta\Big(\sum_{i=1}^{N} n_i(E_i-\mu)\Big)\Big) = \sum_{\{n_i\}} \prod_{i=1}^{N} e^{-\beta n_i(E_i-\mu)} \end{aligned} \tag{1.15}$$

Next, we recall that the system is connected to a reservoir and is much smaller than it. Then, because in the grand canonical ensemble particle exchange is allowed, we can freely assume $N \approx \infty$. Then we can interchange the product with the summation to obtain

$$Z_{gc} = \prod_{i=0}^{\infty} \sum_{n_i=0}^{\infty} e^{-\beta n_i(E_i-\mu)} = \prod_{i=0}^{\infty}(1-ze^{-\beta E_i})^{-1}, \tag{1.16}$$

where we made use of the geometric series formula. The quantity $z = e^{\beta\mu}$ is called **fugacity**. The grand potential then reads

$$\Omega(T,V,\mu) = -\beta \log(Z_{gc}) = \beta \sum_{i=0}^{\infty} \log(1-ze^{-\beta E_i}). \tag{1.17}$$

For the thermal expectation value of the particle number distribution $\langle n_i \rangle$ we have

$$\begin{aligned} \langle n_i \rangle &= -\frac{1}{\beta}\frac{\partial \log Z_{gc}}{\partial E_i} = -\frac{1}{\beta}\frac{1}{1-ze^{-\beta E_i}} z\beta e^{-\beta E_i} \\ &= \frac{1}{z^{-1}e^{\beta E_i}-1}. \end{aligned} \tag{1.18}$$

The Hamiltonian without a potential consists only of the kinetic energy part:

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla_i^2. \tag{1.19}$$

If we further impose periodic boundary conditions in each coordinate direction, the spectrum of H is discrete and given by the quadratic dispersion relation

$$E_{\vec{l}} = \frac{\hbar^2 k^2}{2m} = \frac{4\pi^2\hbar^2|\vec{l}|^2}{2mL^2}, \text{ where } \vec{l} \in \mathbb{Z}^3. \tag{1.20}$$

For the expectation value of the total particle number in the thermodynamic limit we approximate the summation by integration over the phase space to obtain:

$$\begin{aligned} \langle N \rangle &= \sum_{l\in\mathbb{Z}^3} \langle n_l \rangle \xrightarrow[\rho=\mathrm{const}]{L,N\to\infty} \int_{\mathbb{R}^3} \mathrm{d}\mathbf{p} \int_V \mathrm{d}\mathbf{q} n(\mathbf{p}) = \frac{L^3}{(2\pi)^3}\int \mathrm{d}^3\mathbf{p} n(\mathbf{p}) \\ &= \frac{V(2m)^{3/2}}{4\pi^2\hbar^3}\int_0^\infty \mathrm{d}E \frac{\sqrt{E}}{e^{\beta E}z^{-1}-1} = \frac{2V}{\sqrt{\pi}}\frac{1}{\lambda^3}\int_0^\infty \mathrm{d}x \frac{\sqrt{x}}{e^x z^{-1}-1} \\ &=: \frac{V}{\lambda^3} g_{3/2}(z), \end{aligned} \tag{1.21}$$

where $\lambda = \frac{h}{\sqrt{2\pi m\beta^{-1}}}$ is the so-called 'thermal wavelength' of the system and the special function $g(z)$ is defined as

$$g_l(z) := \frac{1}{\Gamma(l)} \int_0^\infty \mathrm{d}x \frac{x^{l-1}}{e^x z^{-1} - 1} = \sum_{n=1}^\infty \frac{z^n}{n^l}. \tag{1.22}$$

This means that the density in the thermodynamic limit is given by

$$\rho(\mu, T) = \frac{1}{\lambda^3} g_{3/2}(z), \tag{1.23}$$

with $z = e^{\beta\mu}$ being the fugacity. Because $g_{3/2}$ is a monotone increasing function in z and thus in μ, the density seems to be bounded from above, as $\mu \to 0$, by

$$\frac{N}{V} = \frac{1}{\lambda^3} g_{3/2}(1) =: \rho_c, \tag{1.24}$$

called the critical density. Since a bounded density is not physical, there must be a flaw in the theory. Using the relation $\beta = 1/k_B T$ with k_B the Boltzmann constant and the temperature dependence of the thermal wavelength λ, equation (1.24) defines a critical temperature for the system given by

$$T_c = \frac{h^2}{2\pi k_B m (\zeta(3/2)\frac{V}{N})^{2/3}}. \tag{1.25}$$

But what happens below T_c and how is it related to the boundedness of ρ?

The flaw comes from the approximation of the sum by an integral, for if more and more particles are going to the ground state as the temperature goes to 0, the density of states is no longer uniformly distributed among the states and is peaked out about E_0. Hence, we have to separate the ground state before taking the thermodynamic limit. This results in

$$\langle N \rangle = \sum_{l \in \mathbb{Z}^3} n_l = n_0 + \sum_{l \in \mathbb{Z}^3 - \{0\}} n_l \approx \frac{1}{z^{-1} - 1} + \frac{1}{\lambda^3} g_{3/2}(z). \tag{1.26}$$

In particular, the number of particles of the ground state is then

$$n_0(T) = \langle N \rangle \Big(1 - \Big(\frac{T}{T_c}\Big)^{3/2}\Big). \tag{1.27}$$

Because of the non-analyticity of $g_l(z)$ at $z = 1$, a phase transition occurs at the critical temperature. We distinguish two phases between the excited fraction of particles n_e and particles in the ground state given by $n_0 = N - n_e$. In a similar fashion we can think of a condensation of a macroscopic number of particles in two or more distinct microscopic states. This phenomenon of macroscopically occupied microscopic state of a system is called 'Bose-Einstein Condensation'.

The equation of state for the non-interacting Bose gas can be obtained from the grand potential using the Gibbs-Duhem relation:

$$-pV = \Omega = \frac{1}{\beta} \log Z_{gc}, \tag{1.28}$$

with the pressure p and the inverse temperature β. Therefore, we obtain the equation

$$\beta p = \frac{1}{V} \log Z_{gc}, \tag{1.29}$$

If we now apply the separation of the ground state in the thermodynamic limit, the grand potential can be computed in a similar manner as the expectation of the total particle number via a continuous approximation of the sum by an integral over phase space. Using the relation $\langle N \rangle = -\frac{\partial \Omega}{\partial \mu}$ and integration by parts, the result is the following equation of state:

$$\frac{p}{k_B T} = \frac{1}{V} \log \frac{1}{1-z} + \frac{1}{\lambda^3} g_{5/2}(z) = \frac{1}{V} \log(n_0 + 1) + \frac{1}{\lambda^3} g_{5/2}(z) \tag{1.30}$$

In the thermodynamic limit, denoted by lim_{TD}, we have $n_0 \sim N$ and therefore

$$\lim_{TD} \frac{1}{V} \log(n_0 + 1) = \lim_{TD} \frac{1}{V} (\log \rho + \log V) = 0. \tag{1.31}$$

Thus, we see that the condensate itself does not contribute to the pressure of the system. Moreover, as more and more particles occupy the ground state, the pressure decreases. This fact is the physical manifestation of the bosonic features discussed in the introduction and clearly cannot hold for fermions due to the Pauli exclusion principle.

Using precisely the same machinery, one can obtain the entropy of the system from the equations of state and show that it vanishes for the condensate. This agrees with the statistical interpretation of entropy as a measure of the disorder of the system, since all bosons occupy the same state, which takes the form of a product of single-particle wave functions.

In comparison to the classical ideal gas, we see that, as the temperature approaches the absolute zero, the quantum nature of particles becomes more pronounced as well. Hence, all equations of state need to be modified in the corresponding regime, to account for the new properties such as pressure and entropy decrease. The system responds to external interaction as one single macroparticle. This reflects true quantum mechanical features in a macroscopic behaviour, which makes the Bose-Einstein condensate extremely interesting.

Chapter 2

The Interacting Bose Gas: The Dilute Limit

2.1 Heuristic Analysis

The analysis in the previous chapter considered the rigorous treatment of the non-interacting Bose gas. The realistic case we want to consider is when a genuine interaction is present. But how does the system behave when we switch on an interaction potential v? A general statement valid for all physical potentials cannot be made, since the solution to the Schrödinger's equation for a system of N particles is out of reach both analytically and numerically, because of the huge number of particles (typically $N \sim 10^{11}$) involved. On the other hand, the physical intuition, based on assuming a smooth response of the system when decreasing the potential to 0, suggests that for a certain class of potentials, the (weakly) interacting gas of bosons exhibits a very similar behaviour to the free gas in a certain limit, to be specified.

A crucial parameter in the analysis of interacting systems is given by the scattering length. It represents an important characteristic value for the effective length scale of the potential and encodes the essential information for the study of scattering:

Theorem 2.1. *Suppose $v \in L^{3/2}(\mathbb{R}^3)$ is spherically symmetric and has finite range, i.e. $v(r) = v(|\boldsymbol{x}|) = 0$ for $r > R_0$ and assume that $\frac{1}{2}v(\boldsymbol{x})$ has no negative energy bound states, i.e.*

$$\int_{\mathbb{R}^3} \mu|\nabla\psi|^2 + \frac{1}{2}v|\psi|^2 \geq 0 \tag{2.1}$$

for all $\psi \in H^1$ and $\mu := \frac{\hbar^2}{2m}$. Further, let $R > R_0$ and let $B_R \subset \mathbb{R}^3$ be the ball about the origin of radius R and $S_R = \partial B_R$ its boundary. For $\psi \in H^1$ set

$$\mathcal{E}_R[\psi] = \int_{B_R} \mu|\nabla\psi|^2 + \frac{1}{2}v|\psi|^2. \tag{2.2}$$

Then there exists a unique $\phi_0 \in \{H^1 : \phi(\boldsymbol{x}) = 1\ \forall \boldsymbol{x} \in S_R\}$ which is nonnegative and spherically symmetric, i.e.

$$\phi_0(\boldsymbol{x}) = \psi_0(|\boldsymbol{x}|) \tag{2.3}$$

with $\psi \geq 0$ on $(0, R]$. Moreover, it satisfies the equation

$$-\mu\Delta\phi_0(\boldsymbol{x}) + \frac{1}{2}v(\boldsymbol{x})\phi_0(\boldsymbol{x}) = 0 \tag{2.4}$$

in the sense of distributions on B_R, with boundary condition $\psi_0(R) = 1$, called the ***zero energy scattering equation****, and*

$$\psi_0(r) = \psi^{asymp}(r) = \frac{1 - a/r}{1 - a/R}, \qquad R_0 < r < R. \tag{2.5}$$

for $|\boldsymbol{x}| = r$ and some constant a, called the ***scattering length****.*

The minimum value of $\mathcal{E}_R[\psi]$ is also given by

$$E = 2\pi^{3/2}\mu a / [\Gamma(3/2)(1 - a/R)]. \tag{2.6}$$

Proof. The proof of the theorem can be found in Appendix C of [13]. It should be mentioned that the conditions on v can be weakened as long as it is a finite, spherically symmetric measure. □

Now, consider a system of N bosons of mass m confined in a cubic box Λ of side length L. Moreover, the particles interact via a spherically symmetric potential $v(|\mathbf{x}_i - \mathbf{x}_j|)$. The Hamiltonian of the system is then given by

$$H_N = -\mu \sum_{i=1}^{N} \Delta_i + \sum_{1 \le i < j \le N} v(|\mathbf{x}_i - \mathbf{x}_j|), \tag{2.7}$$

with the factor $\mu = \frac{\hbar^2}{2m}$. We restrict our attention to nonnegative interaction potentials that decrease faster than $1/r^3$ at infinity. For computational convenience v often will be assumed of compact support, i.e. finite range. Some remarks will be made about extending the theorems to the above case.

Assuming a dilute limit, we are interested in estimating the ground state energy, defined by

$$E_0(N, L) = \inf \left\{ \langle \Psi, H_N \Psi \rangle |\ \Psi \in \bigotimes_{symm}^{N} H^1(\Lambda), \langle \Psi, \sum_{i<j} v(|\mathbf{x}_i - \mathbf{x}_j|)\Psi \rangle < \infty,\ ||\Psi||_2 = 1 \right\}, \tag{2.8}$$

where $H^1(\Lambda)$ denotes the first Sobolev space over the box $\Lambda \subset \mathbb{R}^3$ of side length L. Since we consider bosons only, the wave function should belong to the symmetric product. The notation indicates that in general, before taking the TD-limit, $N \to \infty$, $L \to \infty$, $\rho = N/L^3 = const$, the ground state energy will depend on the parameters N and L and the dependence on the potential in the thermodynamic limit shall turn out to be implicit, through the scattering length a. Hence the theorems and proofs below will be valid for a wide range of potentials, all of them having the same scattering length. The energy per particle in the thermodynamic limit is then given by

$$e_0(\rho, a) := \lim_{L \to \infty} \frac{E_0(\rho L^3, L)}{\rho L^3}. \tag{2.9}$$

The limit above is expected to exist, because of extensivity of the energy.

To define the spectrum of the Hamiltonian H_N unambiguously, we need to specify a boundary condition for the values of Ψ and $\nabla\Psi$ on $\partial\Lambda$. We have that these conditions are all equivalent in the limit, since there is no boundary any more. The easiest choice with respect to the energy is Dirichlet boundary conditions for the upper bound and Neumann boundary conditions for the lower bound, as given in [13].

We now consider the low-density asymptotics of $e_0(\rho, a)$ for dilute gases. Physically, this means that the mean distance between two particles, $\rho^{1/3}$ is much larger than the scattering length, a, of the potential, i.e. we consider only $\rho a^3 \ll 1$. If we take the ball B_R in theorem (2.1) to be of infinite radius, the asymptotic solution to the zero energy scattering equation (2.5) is given by

$$\psi_0(\mathbf{x}) = 1 - \frac{a}{r}, \tag{2.10}$$

for all $r > R_0$. Writing $\psi_0(\mathbf{x}) = u_0(\mathbf{r})/r$, we see that u_0 solves:

$$-2\mu u_0''(r) + v(r)u_0(r) = 0, \tag{2.11}$$

the radial zero-energy equation, with boundary condition $u_0(0) = 0$.

Our main goal in this chapter will be to establish a rigorous proof of the following relation for the energy per particle in the thermodynamic limit:

Theorem 2.2 (Low density limit of the ground state)**.** *Under the assumptions of theorem (2.1) on v and in the low-density limit the following relation holds*

$$\left| \frac{e_0(\rho, a)}{4\pi\mu\rho a} - 1 \right| \xrightarrow{\rho a^3 \to 0} 0. \tag{2.12}$$

To understand (2.12) better, we need to look carefully at the limit above. We have the three natural length scales for the problem: the scattering length a, the inter-particle density $\rho^{1/3}$ and ρa. The last one is proportional to the de Broglie wavelength $l_c \sim (\rho a)^{-1/2}$, sometimes also called 'healing length' or 'uncertainty principle length'. We need to give a physical meaning to l_c. Due to the Heisenberg's uncertainty principle, we can ssociate with the length l_c a momentum $1/l_c = \sqrt{\rho a}$. Physically, using the definition of the kinetic energy, we have $E_{kin} = \frac{p^2}{2m} = \frac{h^2}{2ml_c^2} \sim \rho a$. Then, in the dilute limit, we obtain the following relation:

$$a \ll \rho^{-1/3} \ll l_c. \tag{2.13}$$

The above formula basically relates the inter-particle distance to the de-Broglie wavelength, which is the scale at which the wave nature of particles emerges. Hence, we see that it is not possible to localise the particles with respect to each other without changing their kinetic energy significantly and the condensate shall behave like one whole. Whence, particles lose their individuality completely in the condensate phase.

Let us now try to give a heuristic motivation for (2.12). The energy of a state that solves the zero energy scattering equation ψ_0 in a ball of radius R is given by

$$\begin{aligned} \int_{|\mathbf{x}|\le R} \mu|\nabla\psi_0|^2 + \frac{1}{2}v|\psi_0|^2 &= \oint_{|\mathbf{x}|=R} 2\mu\psi_0\nabla\psi_0 \cdot \vec{n}R^2 \mathrm{d}\omega + \int_{|\mathbf{x}|\le R} \underbrace{(-2\mu\Delta\psi_0 + v\psi_0)}_{\overset{(2.4)}{=}0}\psi_0 \\ &= 8\pi\mu a(1 - \frac{a}{R}) \longrightarrow 8\pi\mu a \end{aligned} \tag{2.14}$$

for $R \to \infty$, where we used integration by parts and the zero order scattering equation. For positive v, ψ_0 minimizes the left-hand side of (2.14) for every $R > R_0$ with boundary condition

$\psi(R) = 1 - a/R$. Now let us first consider two particles only and assume that their wave function is given by

$$\psi(\mathbf{x}, \mathbf{y}) = f(\mathbf{x} - \mathbf{y}, \mathbf{x} + \mathbf{y}),$$

for some $f \in L^2(\Lambda \times \Lambda)$. Observe that the condition $\rho a^3 \to 0$ is equivalent to $a \ll L$. If we further assume a 'soft' interaction potential, $\psi(\mathbf{x}, \mathbf{y})$ is essentially uniform over the box, since the particles are hardly localised with respect to each other. Therefore, the ground state energy is mostly potential. The interaction potential depends on the difference $|\mathbf{x} - \mathbf{y}|$ only. If we set $\mathbf{x} - \mathbf{y} = \eta$, we have $E(2, L) \approx \frac{1}{L^3} \int v(|\eta|) \mathrm{d}\eta$. The prefactor $\frac{1}{L^3}$ comes from the normalisation of the nearly uniform $\psi(\mathbf{x}, \mathbf{y})$. According to [13], perturbation theory is applicable and, in the limit $a \ll L$, $\int v(|\eta|) \mathrm{d}\eta$ is the first Born approximation to $8\pi a\mu$. Altogether we have $E(2, L) \approx 8\pi\mu a/L^3$. A generalisation follows for $N(N-1)/2$ possible interaction pairs. For each particle the total energy estimates to $E_0(N, L) \approx 4\pi\mu a N(N-1)/L^3$, which reduces to (2.12) in the TD limit. It should be mentioned that perturbation theory is valid for 'soft' potentials only. However, (2.12) holds for 'hard' potentials as well. In fact, going from the 'hard' to the 'soft' regime will turn out to be crucial for proving the lower bound.

In the following, we shall prove the theorem rigorously by establishing a lower and an upper bound on the ground state energy. Both of them are non-trivial and require careful examination of the system from a physical point of view, in order to be able to guess a suitable ansatz. The next two subsequent chapters deal with the two bounds.

2.2 The Upper Bound

The upper bound has first been proved by Dyson in 1956 in [3]. Since then, some modifications have been made. In the following, we stick to the proof given by Lieb, Seiringer, Solovej and Yngvason in [13].

Theorem 2.3 (Upper Bound)**.** *Let $\rho_1 = (N-1)/L^3$ and $b = (4\pi\rho_1/3)^{-1/3}$. Further, let v be a non-negative potential, $v \geq 0$, and $b > a$. Then, the ground state energy of (2.7) with periodic boundary conditions satisfies*

$$E_0(N, L) \leq 4\pi\mu\rho_1 a\big(1 + const.\frac{a}{b}\big). \tag{2.15}$$

Hence, in the thermodynamic limit (and for all boundary conditions)

$$\frac{e_0(\rho, a)}{4\pi\mu\rho a} \leq 1 + const.Y^{1/3}, \tag{2.16}$$

for all $Y = 4\pi\rho a^3/3 < 1$.

Proof. We want to establish an upper bound on (2.8). The ground state energy is defined as an infimum and thus any symmetric Ψ will give an upper bound. Since we do not want to restrict ourselves to the symmetric subspace, we make the following observation: H_N, as defined in (2.7), is an elliptic differential operator. Hence, for $v \geq 0$, its lowest eigenvector (the ground state) is a nonnegative function. If we now symmetrise it, it will still have the same energy, since H_N is symmetric under permutations of the particle positions (notice that v dependes on absolute value of the difference of two positions only and every particle interacts with its nearest neighbour). A general proof of this fact is also given in [3]. So we can use any reasonable trial function, even if it violates the symmetry condition, as long as it captures the essential part of the energy. Let us now choose a function of the following form:

$$\Psi(\mathbf{x}_1, ..., \mathbf{x}_N) = F_1(\mathbf{x}_1) \cdot F_2(\mathbf{x}_1, \mathbf{x}_2) \cdots F_N(\mathbf{x}_1, ..., \mathbf{x}_N), \tag{2.17}$$

where $F_1 \equiv 1$ and F_i depends on the distance between $\mathbf{x}_1$ and its nearest neighbour among $\mathbf{x}_1, ..., \mathbf{x}_{i-1}$:

$$F_i(\mathbf{x}_1, ..., \mathbf{x}_i) =: f(t_i), \qquad t_i = \min\{|\mathbf{x}_i - \mathbf{x}_j|, j = 1, ..., i-1\}, \tag{2.18}$$

with a monotone increasing function f, satisfying

$$0 \leq f \leq 1, \qquad f' \geq 0. \tag{2.19}$$

The physical interpretation of the trial function is the following: particles are put into the system one at a time, taking into account the previously inserted ones, but without adjusting the wave function. It clearly does not reflect all the interactions of the ground state, but we shall see that it is sufficient to capture the main term of the energy in the dilute limit.

We now fix the function f to be:

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \leq r \leq b \\ 1 & \text{for } r > b \end{cases} \tag{2.20}$$

with $f_0(r) = u_0(r)/r$ the zero energy scattering solution.

Our goal is first to calculate the quadratic form $\langle \Psi, H_N \Psi \rangle$ of the trial function. To that end, define

$$\varepsilon_{ik} := \begin{cases} 1 & \text{for } i = k, \\ -1 & \text{for } t_i = |\mathbf{x}_i - \mathbf{x}_j|, \\ 0 & \text{otherwise} \end{cases} \tag{2.21}$$

and let $\mathbf{n}_i$ be the unit vector in the direction of $\mathbf{x}_i - \mathbf{x}_{j(i)}$. Here, $\mathbf{x}_{j(i)}$ is the nearest neighbour of $\mathbf{x}_i$ to the points $\mathbf{x}_i - \mathbf{x}_j,\ j = 1, ..., i-1$ and depends not only on i but on the neighbours themselves as well.

We now establish a useful inequality. Consider the identity:

$$\Psi^{-1} \nabla_k \Psi = \sum_i F_i^{-1} \varepsilon_{ik} \mathbf{n}_i f'(t_i). \tag{2.22}$$

To prove it, we first compute

$$\nabla_{x_k} f(t_i) = \nabla_{x_k} f(|\mathbf{x}_i - \mathbf{x}_{j(i)}|) = f'(t_i) \nabla_{x_k} |\mathbf{x}_i - \mathbf{x}_{j(i)}|. \tag{2.23}$$

For the second factor in the above equation we need to distinguish three cases:

- $i = k$: $\nabla_{x_k} |\mathbf{x}_k - \mathbf{x}_{j(k)}| = \nabla_{x_k - x_{j(k)}} |\mathbf{x}_k - \mathbf{x}_{j(k)}| = \mathbf{n}_k$
- $t_i = |\mathbf{x}_i - \mathbf{x}_j|$: $\nabla_{x_k} |\mathbf{x}_i - \mathbf{x}_k| = -\nabla_{x_i - x_k} |\mathbf{x}_i - \mathbf{x}_k| = -\mathbf{n}_k$
- $i \neq k$, $t_i \neq |\mathbf{x}_i - \mathbf{x}_j|$: $\nabla_{x_k} \underbrace{|\mathbf{x}_k - \mathbf{x}_{j(k)}|}_{\text{indep. of } x_k} = 0.$

and we can use the definition of ε_{ik} to write them in a compact way. Further, we insert in (2.23) the definition of Ψ to obtain

$$\begin{aligned}
\Psi^{-1}\nabla_k\Psi &= \Psi^{-1}\nabla_k\prod_{i=1}^{N} f(t_i) = \sum_{i=1}^{N} F_i^{-1}\nabla_{x_k} f(t_i) \\
&= \sum_{i=1}^{N} F_i^{-1}\varepsilon_{ik}\mathbf{n}_i f'(t_i) \qquad (2.24)
\end{aligned}$$

Squaring the left-hand-side of (2.24) and summing over k, we arrive at

$$\begin{aligned}
\Psi^{-2}\sum_k |\nabla_k\Psi|^2 &= \sum_{i,k,j}\varepsilon_{ik}\varepsilon_{jk}\underbrace{\mathbf{n}_i\cdot\mathbf{n}_j}_{\leq 1} F_i^{-1}F_j^{-1}f'(t_i)f'(t_j) \\
\overset{\text{symm in } i,j}{\leq} \; 2\sum_{i<j;\ k}|\varepsilon_{ik}\varepsilon_{jk}|F_i^{-1}F_j^{-1}f'(t_i)f'(t_j) &+ \sum_{i,k}\underbrace{|\varepsilon_{ik}|^2}_{\neq 0 \text{ for } i=k \text{ or } k=j(i)} F_i^{-2}f'^2(t_i) \\
\overset{\nabla_k f(t_i)=0, \text{for } k>i}{=} \; 2\sum_{k\leq i<j}|\varepsilon_{ik}\varepsilon_{jk}|F_i^{-1}F_j^{-1}f'(t_i)f'(t_j) &+ 2\sum_i F_i^{-2}f'^2(t_i) \qquad (2.25)
\end{aligned}$$

Now we are ready to give a first estimate on the expectation of the Hamiltonian:

$$\begin{aligned}
\frac{\langle\Psi, H_N\Psi\rangle}{\langle\Psi,\Psi\rangle} &\leq \underbrace{2\mu\sum_{i=1}^{N}\frac{\int|\Psi|^2F_i^{-2}f'^2(t_i)}{\int|\Psi|^2} + \sum_{1\leq j<i\leq N}\frac{\int|\Psi|^2 v(|\mathbf{x}_i-\mathbf{x}_j)}{\int|\Psi|^2}}_{=I_1} \\
&+ \underbrace{2\mu\sum_{k\leq i<j}\frac{\int|\Psi|^2|\varepsilon_{ik}\varepsilon_{jk}|F_i^{-1}F_j^{-1}f'(t_i)f'(t_j)}{\int|\Psi|^2}}_{=I_2} \qquad (2.26)
\end{aligned}$$

The next goal is to make the i and j dependence of the three terms easy to compute so that we can perform the integrals and eventually cancel what is left of the numerators and the denominators.

Let us now define, for $i<p$, $F_{p,i}$ to be the function F_p if we simply omit particle i as a candidate for a nearest neighbour.

$$F_{p,i}(\mathbf{x}_1,...,\hat{\mathbf{x}}_i,...,\mathbf{x}_p) := f(t_p'), \qquad t_p' = \min\{|\mathbf{x}_i-\mathbf{x}_j|, j=1,...,\hat{\imath},...,p-1\},$$

where $\hat{x}$ stands for omitting the variable x. Hence, $F_{p,i}$ becomes independent of $\mathbf{x}_i$. In the same manner, define $F_{p,ij}$, taking out of consideration $\mathbf{x}_i$ and $\mathbf{x}_i$.

$$F_{p,ij}(\mathbf{x}_1,...,\hat{\mathbf{x}}_i,...,\hat{\mathbf{x}}_j,...,\mathbf{x}_p) := f(t_p''), \qquad t_p'' = \min\{|\mathbf{x}_i-\mathbf{x}_j|, j=1,...,\hat{\imath},...,\hat{\jmath},...,p-1\}.$$

Notice again that $F_{p,ij}$ depends neither on $\mathbf{x}_i$, nor on $\mathbf{x}_j$. Since F_i occurs in the numerator and in the denominator we need estimates from both above and below.

By definition, f is monotone increasing and we have

$$F_p = \min\{F_{p,ij}, f(|\mathbf{x}_p-\mathbf{x}_j|), f(|\mathbf{x}_p-\mathbf{x}_i|)\}. \qquad (2.27)$$

Further, using $0 \leq f \leq 1$ we arrive at

$$\begin{aligned} F_{p,j}^2 f(|\mathbf{x}_p - \mathbf{x}_j|) &\leq F_p^2 \leq F_{p,j}^2 \\ F_{p,ij}^2 f^2(|\mathbf{x}_p - \mathbf{x}_i|) f^2(|\mathbf{x}_p - \mathbf{x}_j|) &\leq F_p^2 \leq F_{p,ij}^2 \end{aligned} \tag{2.28}$$

Observe that the two groups of inequalities above are essentially the same, so we can focus on the second line. The first inequality sign is trivial, since one of the three terms necessarily is equal to the minimum F_p by definition of f and $F_{p,ij}$ and the other two are less or equal to 1. The second inequality sign follows from the fact that omitting the i^{th} and j^{th} particle the minimum in (2.18) is taken over a smaller set, and can therefore only raise.

Consequently, for $j < i$, we obtain the upper bound

$$F_{j+1}^2 \cdots F_{i-1}^2 F_{i+1}^2 \cdots F_N^2 \leq F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,ij}^2 \cdots F_{N,ij}^2. \tag{2.29}$$

To see this, we restrain our attention to the right pair of inequalities in (2.28) and use the first one for $p = j+1, ..., i-1$ and the second one for $p = i+1, ..., N$. Since F is positive, we can just multiply the inequalities. The result yields (2.29).

The lower bound is somehow more tricky, for it involves one more inequality. We follow the same philosophy as above patching together the left pair of inequalities this time. The key ingredient appears to be the Weierstrass product inequality, which holds for $0 \leq f_i \leq 1$ and reads:

$$\prod_{i=1}^N f_i \geq \Big(1 - \sum_{i=1}^N (1 - f_i)\Big). \tag{2.30}$$

It is trivially valid also for f_i^2 since it satisfies the only condition $0 \leq f_i^2 \leq 1$ as well:

$$\begin{aligned} F_j^2 \cdots F_N^2 &\geq F_i^2 F_j^2 F_{j+1,j}^2 f^2(|\mathbf{x}_{j+1} - \mathbf{x}_j|) \cdots F_{i-1,j}^2 f^2(|\mathbf{x}_{i-1} - \mathbf{x}_j) \\ &\times F_{i+1,ij}^2 f^2(|\mathbf{x}_{i+1} - \mathbf{x}_j|) f^2(|\mathbf{x}_{i+1} - \mathbf{x}_i|) \cdots F_{N,ij}^2 \\ &\times f^2(|\mathbf{x}_N - \mathbf{x}_j|) f^2(|\mathbf{x}_N - \mathbf{x}_i|) \\ &= \frac{F_i^2}{f^2(|\mathbf{x}_1 - \mathbf{x}_i|) \cdots f^2(|\mathbf{x}_{i-1} - \mathbf{x}_i|)} \frac{F_j^2}{f^2(|\mathbf{x}_1 - \mathbf{x}_j|) \cdots f^2(|\mathbf{x}_{j-1} - \mathbf{x}_j|)} \\ &\times F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,j}^2 \cdots F_{N,j}^2 \\ &\times f^2(|\mathbf{x}_1 - \mathbf{x}_j|) \cdots f^2(|\mathbf{x}_{j-1} - \mathbf{x}_j|) f^2(|\mathbf{x}_{j+1} - \mathbf{x}_j|) \cdots f^2(|\mathbf{x}_{i-1} - \mathbf{x}_j|) \\ &\times f^2(|\mathbf{x}_{i+1} - \mathbf{x}_j|) \cdots f^2(|\mathbf{x}_N - \mathbf{x}_j|) \times f^2(|\mathbf{x}_1 - \mathbf{x}_i|) \cdots \\ &\times f^2(|\mathbf{x}_{i-1} - \mathbf{x}_i|) f^2(|\mathbf{x}_{i+1} - \mathbf{x}_i|) \cdots f^2(|\mathbf{x}_N - \mathbf{x}_i|) \\ &\geq F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,j}^2 \cdots F_{N,j}^2 \prod_{k=1;k\neq i}^N f^2(|\mathbf{x}_i - \mathbf{x}_k|) \prod_{k=1;k\neq i,j}^N f^2(|\mathbf{x}_j - \mathbf{x}_k|) \\ &\geq F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,j}^2 \cdots F_{N,j}^2 \\ &\times \underbrace{\Big(1 - \sum_{k=1;k\neq i}^N (1 - f^2(|\mathbf{x}_i - \mathbf{x}_k|))\Big)}_{=:A} \underbrace{\Big(1 - \sum_{k=1;k\neq i,j}^N (1 - f^2(|\mathbf{x}_j - \mathbf{x}_k|))\Big)}_{=:B}. \end{aligned} \tag{2.31}$$

Several factors have artificially been added to the product. To estimate the F_j and F_i fractions, notice that the numerators, defined as minimum, are always taken by one of the factors on the denominators, respectively, so they will be cancelled and what is left in the denominators is less than 1 by properties of f. Hence, both fractions are greater or equal to 1.

We continue developing our machinery by noticing the following estimate on the derivative f':

$$f'^2(t_i) \leq \sum_{j=1}^{i-1} f'^2(\mathbf{x}_i - \mathbf{x}_j), \tag{2.32}$$

which follows immediately from $f' \geq 0$ and the definition of t_i.

We shall also need an estimate on the integral below, which follows from the positivity of the integrand:

$$\int_\Lambda \mu(f'(r))^2 + \frac{1}{2}v(r)f^2(r)\mathrm{d}\mathbf{x} \leq \frac{1}{2}\int_{r\leq b} 2\mu f'^2(r) + v(r)f^2(r) \overset{(2.14)}{=} 4\pi a\mu\big(1-\frac{a}{b}\big)f_0^{-2}(b) \tag{2.33}$$

By a property of the asymptotic solution to the zero order scattering equation, proved in Appendix C of [13], we have $f_0(b) \geq 1 - a/b$. Hence, we obtain

$$\int_{\Lambda^2} 2\mu f'^2(\mathbf{x}_i - \mathbf{x}_j) + v(|\mathbf{x}_i - \mathbf{x}_j|)f^2(\mathbf{x}_i - \mathbf{x}_j)\mathrm{d}\mathbf{x}_i\mathrm{d}\mathbf{x}_j \leq 8\pi a\mu L^3(1-a/b)^{-1} \tag{2.34}$$

The last inequality we need before estimating (2.26) further is

$$\begin{aligned} A = \int_\Lambda \left[1 - \sum_{k=1;k\neq i}^{N}(1 - f^2(|\mathbf{x}_i - \mathbf{x}_k|))\right]\mathrm{d}\mathbf{x}_i \ &\geq\ L^3 - \sum_{k=1;k\neq i}^{N}\int_{\mathbb{R}^3}(1 - f^2(|\mathbf{x}_i - \mathbf{x}_k|)) \\ &\geq\ L^3 - (N-1)I \end{aligned} \tag{2.35}$$

where A is defined in (2.31) and I is given by $I = \int_{\mathbb{R}^3}(1 - f^2(r))\mathrm{d}\mathbf{x}$. Here we made use of the fact that the integrand is nonnegative and thus, enlarging the integration domain can only make the integral bigger, and hence the total expression smaller. Exactly the same argument applies to show that

$$B \geq L^3 - (N-2)I \geq L^3 - (N-1)I, \tag{2.36}$$

with B defined in (2.31) as well.

Now, we are equipped with everything we need to estimate the integrals I_1 and I_2. Let us not concern with the denominators for the moment. We begin by considering I_1 and plugging in the definition for Ψ in the numerators. In the kinetic energy term of I_1 a factor F_i^2 will cancel the present F_i^{-2} and we can estimate from above $F_j^2 \leq 1$. In the potential term, we single out $F_i^2 = f^2(t_i)$ and again sacrifice $F_j^2 \leq 1$. Monotonicity yields $f^2(t_i) \leq f^2(|\mathbf{x}_i - \mathbf{x}_j|)$, since $j < i$. Now, using (2.32), we can combine both terms to obtain

$$
\begin{aligned}
I_1 \quad &\leq \quad \sum_{i=1}^{N} \frac{\int \Big\{ F_1^2 \cdots F_{j-1}^2 F_{j+1}^2 \cdots F_{i-1}^2 F_{i+1}^2 \cdots F_N^2}{\int \Big\{ F_1^2 \cdots F_{j-1}^2} \\
&\qquad \frac{\big(\sum_{k=1}^{i-1} 2\mu f'^2(|\mathbf{x}_i - \mathbf{x}_k|) + v(|\mathbf{x}_i - \mathbf{x}_k) f^2(|\mathbf{x}_i - \mathbf{x}_k|)\big)\Big\}}{F_j^2 \cdots F_N^2 \Big\}} \\
&\overset{(2.29),(2.31)}{\leq} \sum_{i=1}^{N} \frac{\int \Big\{ F_1^2 \cdots F_{j-1}^2 F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,ij}^2 \cdots F_{N,ij}^2}{\int \Big\{ F_1^2 \cdots F_{j-1}^2} \\
&\qquad \frac{\big(\sum_{k=1}^{i-1} 2\mu f'^2(|\mathbf{x}_i - \mathbf{x}_k|) + v(|\mathbf{x}_i - \mathbf{x}_k) f^2(|\mathbf{x}_i - \mathbf{x}_k|)\big)\Big\}}{F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,j}^2 \cdots F_{N,j}^2 AB \Big\}} \\
&\overset{(2.34),(2.35)}{\leq} \sum_{i=1}^{N} \frac{\int F_1^2 \cdots F_{j-1}^2 F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,ij}^2 \cdots F_{N,ij}^2 \big(\sum_{j=k}^{i-1} 8\pi a\mu L^3 (1-a/b)^{-1}\big)}{\int F_1^2 \cdots F_{j-1}^2 F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,j}^2 \cdots F_{N,j}^2 [L^3 - (N-1)I]^2} \\
&= \quad \sum_{i=1}^{N} \sum_{j=k}^{i-1} \frac{8\pi a\mu L^3 (1-a/b)^{-1}}{[L^3 - (N-1)I]^2} = \frac{N(N-1)}{2L^3} \frac{8\pi a\mu}{(1-a/b)} \frac{1}{[1 - \frac{N-1}{L^3} I]^2} \\
&= \quad \frac{4\pi a\mu \rho_1 N}{(1-a/b)(1-\rho_1 I)^2}
\end{aligned}
\tag{2.37}
$$

The crucial step has been done in the second inequality, noticing that the $\mathbf{x}_i$ and the $\mathbf{x}_j$ integration can be carried out independently both in the denominator and the numerator due to the definition of $F_{p,ij}$ and irrespectively of the functions F. To complete our estimate on I_1, we need an upper bound on I itself:

$$
\begin{aligned}
I &= \int_{\mathbb{R}^3} \big[1 - f^2(r)\big]\, \mathrm{d}\mathbf{x} \overset{f=1, \text{ for } r>b}{=} 4\pi \int_0^b (1 - f^2(r)) r^2 \mathrm{d}r \\
&\leq 4\pi \int_0^b (1 - f_0^2(r)/f_0^2(b)) r^2 \mathrm{d}r \overset{f_0(r) \geq [1-a/r]_+}{\leq} 4\pi \int_0^b \mathrm{d}r r^2 - \frac{(r-a)^2}{(b-a)^2} b^2 \\
&= \frac{4\pi}{3} \Big[b^3 - \frac{b^2}{(b-a)^2}((b-a)^3 + a^3) \Big] \leq \frac{4\pi}{3} ab^2
\end{aligned}
\tag{2.38}
$$

Altogether, using $b^3 = (4\pi\rho_1/3)^{-1}$, we obtain the following bound:

$$
I_1 \leq N 4\pi \rho_1 \mu a (1 + O(b/a)).
\tag{2.39}
$$

The integral I_2 is estimated in a similar fashion:

$$
\begin{aligned}
I_2 \quad &= \quad 2\mu \sum_{k \leq i < j}^{N} \frac{\int F_1^2 \cdots F_{j-1}^2 F_{j+1}^2 \cdots F_{i-1}^2 F_{i+1}^2 \cdots F_N^2 |\varepsilon_{ik} \varepsilon_{jk}| F_i^{-1} F_j^{-1} f'(t_i) f'(t_j)}{\int F_1^2 \cdots F_{j-1}^2 F_j^2 \cdots F_N^2} \\
&\overset{(2.29),(2.31)}{\leq} 2\mu \sum_{i<j}^{N} \int \frac{F_1^2 \cdots F_{j-1}^2 F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,ij}^2 \cdots F_{N,ij}^2 \sum_{k \leq i} \tilde{K}_k}{\int F_1^2 \cdots F_{j-1}^2 F_{j+1,j}^2 \cdots F_{i-1,j}^2 F_{i+1,j}^2 \cdots F_{N,j}^2 AB}
\end{aligned}
\tag{2.40}
$$

where

$$\tilde{K}_k = \int \mathrm{d}\mathbf{x}_i \mathrm{d}\mathbf{x}_j |\varepsilon_{ik}| F_i f'(t_i) |\varepsilon_{jk}| F_j f'(t_j) \tag{2.41}$$

We now perform the integration over $\mathbf{x}_j$ first. The factor $\varepsilon_{jk} = 0$, unless $j = k$ or $t_j = |\mathbf{x}_j - \mathbf{x}_k|$. The first is, however, excluded by the restriction on the summation. But then we have

$$\begin{aligned}
\sum_{k\le i} \tilde{K}_k &= \sum_{k\le i} \int \mathrm{d}\mathbf{x}_i |\varepsilon_{ik}| F_i f'(t_i) \underbrace{\int \mathrm{d}\mathbf{x}_j f(|\mathbf{x}_j - \mathbf{x}_k|) f'(|\mathbf{x}_j - \mathbf{x}_k|)}_{:=K} \\
&= K \sum_{k\le i} \int \mathrm{d}\mathbf{x}_i |\varepsilon_{ik}| F_i f'(t_i) = 2K \int \mathrm{d}\mathbf{x}_i f(t_i) f'(t_i) \\
&\overset{(2.32)}{\le} \sum_{n=1}^{i-1} \int \mathrm{d}\mathbf{x}_i f(|\mathbf{x}_i - \mathbf{x}_n|) f'(|\mathbf{x}_i - \mathbf{x}_n|) \\
&= 2(i-1)K^2,
\end{aligned} \tag{2.42}$$

since $\varepsilon_{ik} \neq 0$ only for two values of k. Then I_2, after inserting the estimates on A and B and cancelling the remaining terms in the numerator and the denominator, reduces to

$$I_2 \le \frac{2\mu K^2 \sum_{i\le j}^N 2(i-1)}{[L^3 - (N-1)I]^2} \le \frac{1}{3} N(N-1)(N-2) \frac{2\mu K^2}{[L^3 - (N-1)I]^2} \tag{2.43}$$

Next, we calculate K, using the specific form of f given in equation (2.20):

$$\begin{aligned}
K &= \int_{\mathbb{R}^3} f(r) f'(r) \mathrm{d}\mathbf{x} \overset{f'=0,\ \text{for } r>b}{=} 4\pi \int_{r\le b} \underbrace{f(r)}_{\le 1} f'(r) \mathrm{d}\mathbf{x} \\
&\overset{f'=\frac{a}{r^2} f_0^{-1}(b)}{\le} 4\pi \int_0^b \mathrm{d}r r^2 \frac{a}{1-a/b} \frac{1}{r^2} = 4\pi \frac{ab}{1-a/b}
\end{aligned} \tag{2.44}$$

Altogether, recalling the definition $b^3 = (4\pi\rho_1/3)^{-1}$ once again, this yields

$$I_2 \le \text{const.} \rho_1 \mu a \frac{a}{b} \tag{2.45}$$

Combining the bounds on I_1 and I_2 finally proves the upper bound.

□

2.3 The Lower Bound

The lower bound for the energy functional is highly non-trivial and contains some very important insights. One particular reason for this is the presence of three different length scales that play a significant role throughout the proof:

- The scattering length a.
- The mean particle distance $\rho^{-1/3}$.
- The 'uncertainty' principle length l_c, defined in the introduction.

The following theorem can be found in [13].

Theorem 2.4. ***(Lower bound in the TD limit)*** *Let v be a positive potential of finite range. Then for $Y = \frac{4\pi\rho a^3}{3}$*

$$\frac{e_0(\rho, a)}{4\pi\mu\rho a} \geq (1 - CY^{1/17}) \tag{2.46}$$

with C some constant.

For potentials v of no compact support but decreasing faster than $1/r^3$ at infinity there is a similar statement for the ground state energy with $CY^{1/17}$ replaced by $o(1)$ as $Y \to 0$. Moreover, the error term in (2.46) is considered to have no physical meaning. The constant C can be taken to be 8.9 [29]
The next theorem (also from [13]) considers a dilute Bose gas in a box of side length L and fixed number of particles N. Its importance is revealed in application to inhomogeneous dilute systems as discussed in the next chapter.

Theorem 2.5. ***(Lower bound in a finite box)*** *For any $v \geq 0$ of finite range there exists a $\delta > 0$ such that the ground state energy of (2.7) with Neumann boundary conditions satisfies*

$$E_0(N, L)/N \geq 4\pi\mu\rho a(1 - CY^{1/17}) \tag{2.47}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$ and some positive constants C and C', independent of N and L.

As previously remarked, a similar bound also holds if v does not have finite range but decays sufficiently fast at infinity.

The proof of the above theorem begins with a generalisation of a lemma by Dyson. The idea is to increase the effective range of the potential which leads to decrease in the kinetic energy of the system. To do this, it suffices to reduce the L^∞ norm of v without changing the total energy much.

Lemma 2.6 (Dyson)**.** *Let $v(r) \geq 0$ have finite range R_0 and let $U(r) \geq 0$ be any function satisfying $\int U(r) r^2 \mathrm{d}r \leq 1$ and $U(0) = 0$ for $r < R_0$. Let also $\mathcal{B} \subset \mathbb{R}^3$ be star-shaped with respect to 0. Then for all differentiable functions ψ*

$$\int_{\mathcal{B}} (\mu|\nabla\psi|^2 + \frac{1}{2} v|\psi|^2) \geq \mu a \int_{\mathcal{B}} U|\psi|^2. \tag{2.48}$$

Proof. It suffices to prove (2.48) for $\mu|\nabla\psi|^2$ replaced by $\mu|\frac{\partial\psi}{\partial r}|^2$ along the lines of constant angular variables. Then $\psi(\mathbf{x}) = u(r)/r$ with $u(0) = 0$ follows from the solution of the zero energy scattering equation. Consider first the special case

$$U(r) = \frac{1}{R^2}\delta(r - R) \tag{2.49}$$

for some $R \geq R_0$. Along any radial line (2.48) reduces to:

$$\int_0^{R_1} \{\mu[u'(r) - (u(r)/r)]^2 + \frac{1}{2} v(r)|u(r)|^2\}\mathrm{d}r \geq \left\{ \begin{array}{ll} 0 & \text{if } R_1 < R \\ \mu a|u(R)|^2/R^2 & \text{if } R \leq R_1 \end{array} \right. \tag{2.50}$$

with R_1 the length of the radial line segment in $\mathcal{B}$. For $R_1 < R$ the positivity of v yields $\mu|\frac{\partial\psi}{\partial r}|^2 + \frac{1}{2}v|\psi|^2 \geq 0$, establishing the first case. For $R \leq R_1$ we minimise the functional with respect to u under the boundary condition $u(0) = 0$. By homogeneity, we can normalize u so that $u(R) = R - a$. Using the Euler-Lagrange equations, one gets $2\mu[u'' - u/r^2] + v(r)u = 0$ which is precisely the zero energy scattering equation. By assumption, $v \geq 0$ and thus the solution is a true minimum.

Since $v = 0$ for $r > R_0$, the solution u_0 satisfies $u_0(r) = r - a$ for $r > R_0$. Then

$$
\begin{aligned}
\int_0^R \{\mu[u'(r) - \big(u(r)/r\big)]^2 + \frac{1}{2}v(r)|u(r)|^2\} &= \int_0^R \left[\mu\partial_r \frac{u_0}{r} r^2 \partial_r \frac{u_0}{r} + \frac{1}{2}v|u_0|^2\right] \\
= \mu\frac{u_0}{r}r^2\partial_r\Big(\frac{u_0}{r}\Big)\Big|_0^R - \int_0^R \mu\frac{u_0}{r}\,\underbrace{\partial_r\, \underbrace{r^2\partial_r\frac{u_0}{r}}_{=ru_0'-u_0}}_{=u_0''r} + \frac{1}{2}v|u_0|^2 &= \mu\frac{|R-a|}{R}R^2\frac{a}{R^2} - \int_0^R \underbrace{[\mu u_0'' - \frac{1}{2}vu_0]}_{=0}\,u_0 \\
= \mu a\frac{|R-a|}{R} &\geq \mu a\frac{(R-a)^2}{R^2}
\end{aligned}
\tag{2.51}
$$

where integration by parts has been used. But the RHS of the above equation is exactly what is needed, taking into account the normalisation condition.

The general case then follows from the fact that any $U(r)$ may be written as a superposition $U(r) = \int R^{-2}\delta(r-R)U(R)R^2\mathrm{d}r$ of δ-functions and $\int U(R)R^2 \leq 1$, thereby concluding the proof of the Lemma. □

The following corollary arises in a natural way, we dividing the big box Λ for given $\mathbf{x}_1, ..., \mathbf{x}_N$ into Voronoi cells $\mathcal{B}_i$:

Corollary 2.7. *For any U as in Lemma 2.6*

$$H_N \geq \mu a W_R \tag{2.52}$$

as operators, with W being the multiplication operator

$$W_R(\boldsymbol{x}_1, ..., \boldsymbol{x}_N) := \sum_{i=1}^N U(t_i), \tag{2.53}$$

where t_i is the distance of x_i to its nearest neighbour among the x_j's, $j = 1, ..., N$,i.e.

$$t_i(\boldsymbol{x}_1, ..., \boldsymbol{x}_N) = \min_{j, j\neq i} |\boldsymbol{x}_i - \boldsymbol{x}_j| \tag{2.54}$$

In the following we use a specific form of the potential U which turns out to be sufficient for the upcoming estimates:

$$U(r) = \begin{cases} 3(R^3 - R_0^3) & \text{for } R_0 < r < R \\ 0 & \text{otherwise} \end{cases} \tag{2.55}$$

We now use the Lemma 2.6 to go to the 'soft potential regime' sacrificing a part of the kinetic energy. We remark that it is crucial not to sacrifice all of it.(cf. [13], p. 20 for a more detailed discussion). Thus, for $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1-\varepsilon)H_N \geq \varepsilon T_N + (1-\varepsilon)H_N, \tag{2.56}$$

since $v \geq 0$, where $T_N = -\mu \sum_i \Delta_i$. Now we use Corollary 2.7 only for the second part above, obtaining:

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu a W_R. \tag{2.57}$$

We want to consider the second operator on the right-hand-side, denoted by V, as a small perturbation to $H_0 = \varepsilon T_N$. The normalized ground state of H_0 in a box of length L is given by $\Psi_0(\mathbf{x}_1, ..., \mathbf{x}_N) = L^{-3/2}$ and let us denote the expectation value in this state by $\langle \cdot \rangle_0$. A straightforward calculation (cf. [16]) gives:

$$\begin{aligned} 4\pi\rho(1-1/N) &\geq a\frac{\langle W_R\rangle_0}{N} \\ &\geq 4\pi\rho\Big(1-\frac{1}{N}\Big)\Big(1-\frac{2R}{L}\Big)^3\Big(1+4\pi\rho\frac{(R^3-R_0^3)}{3}\Big)^{-1}. \end{aligned} \tag{2.58}$$

The factors have the following interpretation: $(1-\frac{1}{N})$ represents the number of pairs which amounts to $N(N-1)/2$; $(1-\frac{2R}{L})^3$ is due to the fact that the interaction beyond the boundary of Λ is disregarded, while the last factor gives the probability of finding a particle within the interaction range of U_R.

Our next goal shall be to establish rigorous error terms, possibly depending on ε, R and L. To this end we recall Temple's inequality for the expectations of an operator $H = H_0 + V$:

Lemma 2.8. ***(Temple's Inequality)*** *Let E_0, E_1 be the two lowest eigenvalues of the self-adjoint operator H and assume that $E_0 < E_1$ and $E_1 - \langle H\rangle_0 > 0$. Then*

$$E_0 \geq \langle H\rangle_0 - \frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0}. \tag{2.59}$$

Proof. Consider the inequality $(H-E_0)(H-E_1) \geq 0$ of operators. To prove it, notice first that the operators $(H-E_0)$ and $(H-E_1)$ are self-adjoint. $(H-E_0)(H-E_1)$ projects out the two eigenstates corresponding to the two lowest eigenvalues E_0 and E_1 of H and it is sufficient to prove the above inequality for the subspace $span\{\Psi_0,\ \Psi_1\}^\perp \subset span\{\Psi_0\}^\perp$. Here Ψ_i represents the eigenvector of H corresponding to the eigenvalue E_i. Since $(H-E_0)$ commutes with $(H-E_1)$ and $(H-E_0)$ is positive we can take the square root to arrive at

$$\begin{aligned} \langle\Psi,(H-E_0)(H-E_1)\Psi\rangle &= \langle\Psi,\sqrt{(H-E_0)}(H-E_1)\sqrt{(H-E_0)}\Psi\rangle \\ &= \langle\sqrt{(H-E_0)}^*\Psi,(H-E_1)\sqrt{(H-E_0)}\Psi\rangle \\ &= \langle\sqrt{(H-E_0)}\Psi,(H-E_1)\sqrt{(H-E_0)}\Psi\rangle \\ &= \langle\Phi,(H-E_1)\Phi\rangle \geq 0. \end{aligned} \tag{2.60}$$

Notice that the above inequality is valid for all Φ in the range of $\sqrt{(H-E_0)}$, since $(H-E_1)$ is positive on $ran\sqrt{(H-E_0)}$ (the only subspace where $(H-E_1)$ is negative is the one corresponding to E_0 but it is projected out by $\sqrt{(H-E_0)}$).

Let us now return to the proof of Temple's inequality. In particular, it follows for $\Psi = \Psi_0$:

$$\begin{aligned} \langle\Psi_0,(E_0-H)(E_1-H)\Psi_0\rangle &= \langle(E_0-H)\Psi_0,(E_1-H)\Psi_0\rangle \\ &= \langle E_0\Psi_0,(E_1-H)\Psi_0\rangle - \langle H\Psi_0,(E_1-H)\Psi_0\rangle \\ &= E_0E_1\langle\Psi_0,\Psi_0\rangle - E_0\langle H\rangle_0 - E_1\langle H\rangle_0 + \langle H^2\rangle_0 \\ &= E_0(E_1-\langle H\rangle_0)\underbrace{-E_1\langle H\rangle_0 + \langle H\rangle_0^2}_{-\langle H\rangle_0(E_1-\langle H\rangle_0)} + (\langle H^2\rangle_0 - \langle H\rangle_0^2) \\ &\geq 0. \end{aligned} \tag{2.61}$$

But then, using the two assumptions, we simply rearrange terms to finish the proof of the Lemma:

$$\begin{aligned}(E_0 - \langle H\rangle_0)(E_1 - \langle H\rangle_0) &\geq -(\langle H^2\rangle_0 - \langle H\rangle_0^2)\\ (E_0 - \langle H\rangle_0) &\geq -\frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0}\\ E_0 &\geq \langle H\rangle_0 - \frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0}. \end{aligned} \tag{2.62}$$

□

Moreover, since for $V \geq 0$ we have $E_1 \geq E_1^0$, the second eigenvalue of H_0, we can also replace E_1 by E_1^0. Now, recalling the definitions of H_0 and V, we have for $H = H_0 + V$:

$$\langle H\rangle_0 = (1-\varepsilon)\mu a\langle W_R\rangle_0 \tag{2.63}$$

$$\langle H\rangle_0^2 = (1-\varepsilon)^2\mu^2 a^2\langle W_R\rangle_0^2 \tag{2.64}$$

$$\langle H^2\rangle_0 = \langle H_0^2 + V^2 + H_0V + VH_0\rangle_0 = \langle V^2\rangle_0 = (1-\varepsilon)^2\mu^2a^2\langle W_R^2\rangle_0 \tag{2.65}$$

where we several times made use of the fact that $H_0\Psi_0 = 0$, since Ψ_0 is constant. Now, we plug in these relations into the estimate (2.58) to obtain

$$E_0 \geq (1-\varepsilon)\mu a\langle W_R\rangle_0 - \frac{(1-\varepsilon)^2\mu^2a^2(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2)}{E_1^0 - (1-\varepsilon)\mu a\langle W_R\rangle_0} \tag{2.66}$$

Next, we take a prefactor in front of the brackets and divide the whole expression by N to arrive at:

$$\frac{E_0}{N} \geq (1-\varepsilon)\mu a\frac{\langle W_R\rangle_0}{N}\Big(1 - \frac{(1-\varepsilon)\mu a(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2)}{\langle W_R\rangle_0(E_1^0 - (1-\varepsilon)\mu a\langle W_R\rangle_0)}\Big) \tag{2.67}$$

Since $\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2 = (\langle H - \langle H\rangle_0\rangle_0)^2 \geq 0$, taking into account $\varepsilon < 1$, we can drop the ε from both the numerator and the denominator of the right term in the brackets:

$$\frac{E_0}{N} \geq (1-\varepsilon)\mu a\frac{\langle W_R\rangle_0}{N}\Big(1 - \frac{\mu a(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2)}{\langle W_R\rangle_0(E_1^0 - \mu a\langle W_R\rangle_0)}\Big). \tag{2.68}$$

Now, let us set for simplicity

$$1 - \mathcal{E}(\rho, L, R, \varepsilon) = (1-\varepsilon)\frac{\langle W_R\rangle_0}{N}\Big(1 - \frac{\mu a(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2)}{\langle W_R\rangle_0(E_1^0 - \mu a\langle W_R\rangle_0)}\Big) \tag{2.69}$$

and work further with the relation:

$$\frac{E_0}{N} \geq 4\pi\mu a\rho(1 - \mathcal{E}(\rho, L, R, \varepsilon)). \tag{2.70}$$

The next proposition gives an upper bound on the expectation value of the square of the effective potential $\langle W_R^2\rangle_0$ and will be used later on in the proof:

Proposition 2.9.

$$\langle W_R^2\rangle_0 \leq \frac{3N}{R^3 - R_0^3}\langle W_R\rangle_0. \tag{2.71}$$

Proof. Since $W_R = \sum_{i=1}^N U_R(t_i)$, it follows that $W_R^2 = \sum_{i,j=1}^N U_R(t_i)U_R(t_j)$. But then, using that any multiplication operator can be put on either side of the scalar product, we have:

$$\begin{aligned}
\langle W_R^2 \rangle_0 &= \langle \Psi_0, W_R^2 \Psi_0 \rangle \\
&= \sum_{i,j=1}^N \langle U(t_i)\Psi_0, U(t_j)\Psi_0 \rangle \overset{Schwarz}{\leq} N \sum_{i=1}^N ||\Psi_0 U_R(t_i)||^2 \\
&= N\langle \Psi_0, \sum_i U_R^2(t_i)\Psi_0 \rangle \leq \frac{3N}{R^3 - R_0^3} \langle \Psi_0, \sum_i \Psi_0 \rangle \\
&= \frac{3N}{R^3 - R_0^3} \langle W_R \rangle_0. \qquad (2.72)
\end{aligned}$$

□

If we take a closer look at the error term in (2.70), we see that it is here not possible to take the limit $L \to \infty$ with ρ held fixed, since for the energy of the first excited state of the unperturbed one-particle Hamiltonian in a box we have $E_1^0 = \varepsilon \pi^2 \mu / L^2$. Thus, the factor $E_1^0 - \mu a \langle W_R \rangle_0)$ in the denominator of the second term in (2.69) is proportional to $(\varepsilon L^{-2} - a\rho^2 L^3)$ and for L large, the denominator could become negative, whence Temple's inequality could be violated.

The rescue comes from an idea by Lieb and Yngvason [18] called 'the cell method': we divide the big box Λ into cubic cells of side length l that is eventually kept fixed as $L \to \infty$. This means that the number of small boxes L^3/l^3 will grow with L. On each small box we impose Neumann boundary conditions, to keep the energy as low as possible. The particles themselves will be randomly distributed among the cells. However, interaction of particles in contiguous cells will be neglected - which can only lower the ground state energy of the gas due to the non-negativity of the potential. In the end, we have to minimise over all possible distributions of particles, keeping the total particle number N fixed.

Mathematically the cell method is equivalent to the estimate

$$E_0(N, L)/N \geq (\rho l)^{-1} \inf_{\{c_n \geq 0\}} \sum_{n \geq 0} c_n E_0(n, l) \qquad (2.73)$$

under the constraints

$$\sum_{n \geq 0} c_n = 1 \qquad \sum_{n \geq 0} n c_n = \rho l^3. \qquad (2.74)$$

Observe that the ground state energy $E_0(n, l)$ is superadditive, i.e.

$$E_0(n + n', l) \geq E_0(n, l) + E_0(n', l). \qquad (2.75)$$

This is easily seen by dropping the interactions between the n and the n' particles (again using the positivity of v). Furthermore, it follows from the above property that for any n, $p \in \mathbb{N}$ with $n \geq p$

$$E_0(n, l) \geq [n/p] E_0(p, l) \geq \frac{n}{2p} E_0(p, l) \qquad (2.76)$$

since the largest integer $[n/p]$ smaller than n/p is always $\geq n/(2p)$. Now let us go back to the lower bound (2.70) and replace L by l, N by n and ρ by n/l^3. Then, for fixed R and ε we have

$$E_0(n, l) \geq \frac{4\pi\mu a}{l^3} n(n-1) K(n, l) \qquad (2.77)$$

for a function $K(n,l)$ defined by

$$K(n,l) = l^3(1 - \mathcal{E}(\rho, L, R, \varepsilon)).$$

It will soon be shown that K is a monotone decreasing function of n, so for any $p \in \mathbb{N}$ with $n \leq p$ we obtain

$$E_0(n,l) \geq \frac{4\pi\mu a}{l^3} n(n-1)K(p,l). \tag{2.78}$$

Let us now consider the sum under the infimum in (2.73) and divide it in two. For $n < p$ we use (2.78), for $n \geq p$ (2.76), and again (2.78) for $n = p$. The goal is to minimise the expression

$$\sum_{n<p} c_n n(n-1) + \frac{1}{2}\sum_{n \geq p} c_n n(p-1) \tag{2.79}$$

subject to the constraints (2.74). Substituting $k := \rho l^3$ and $t := \sum_{n<p} c_n n \leq k$ we have $\sum_{n \geq p} c_n n = k - t$ and $k := \sum_{n \geq 0} c_n n$ Convexity of $n(n-1)$ in n yields:

$$\sum_{n<p} c_n n(n-1) \geq \sum_{n<p} c_n n \Big(\sum_{n<p} c_n n - 1 \Big) = t(t-1). \tag{2.80}$$

Thus, we have just obtained that (2.79)$\geq t(t-1) + \frac{1}{2}(k-t)(p-1)$. Minimising for $1 \leq t \leq k$, we find the minimum at $t = k$ for $p \geq 4k$ to take the value $k(k-1)$. Putting everything together yields:

$$\frac{E_0(N,L)}{N} \overset{K \text{ mon. decr.}}{\geq} 4\pi\mu a\rho\Big(1 - \frac{1}{\rho l^3}\Big)K(4\rho l^3, l). \tag{2.81}$$

Now, let us inspect $K(4\rho l^3, l)$ more carefully. It depends on the parameters ε, R and l which need to be chosen in an optimal way. From (2.69), dropping the second expectation value in the numerator of the second term in the brackets, and from Proposition 2.9, cancelling the $\langle W_R \rangle_0$ from both the new numerator and the denominator, we obtain

$$K(n,l) \geq A\left(1 - \frac{\frac{3n\mu a}{R^3 - R_0^3}}{\frac{\varepsilon\pi^2\mu}{l^2} - \mu a\langle W_R\rangle_0}\right) = A\left(1 - \frac{3na}{(R^3 - R_0^3)(\epsilon\pi^2 l^{-2} - a\langle W_R\rangle_0)}\right) \tag{2.82}$$

for a prefactor A given by

$$A = (1-\varepsilon)\left(1 - \frac{2R}{l}\right)^3\left(1 + \frac{4\pi}{3}(R^3 - R_0^3)\right)^{-1}.$$

Next, we need the upper bound $\langle W_R \rangle_0 \leq n4\pi\rho(1 - 1/n) = \frac{4\pi n}{l^3}(n-1)$, obtained in (2.58). Finally, we arrive at

$$\begin{aligned} K(n,l) \quad \geq \quad & (1-\varepsilon)\Big(1 - \frac{1}{N}\Big)\Big(1 - \frac{2R}{L}\Big)^3\Big(1 + 4\pi\rho\frac{(R^3 - R_0^3)}{3}\Big)^{-1} \\ \times \quad & \Big(1 - \frac{3}{\pi}\frac{na}{(R^3 - R_0^3)(\varepsilon\pi l^{-2} - 4al^{-3}n(n-1)}\Big). \end{aligned} \tag{2.83}$$

We remark that estimate (2.83) is correct if the denominator in the last factor is positive. We can take 0 as a trivial lower bound whenever (2.78) becomes negative. More importantly, we see that $K(n,l)$ is indeed monotone decreasing in n.

Inserting $n = 4\rho l^3$, setting $Y := 4\pi\rho a^3/3$ and taking into account the prefactor of (2.81): $1 - 1/(\rho l^3) = 1 - (const.)Y^{-1}(a/l)^3$, we finally arrive at

$$\begin{aligned} \frac{E_0(N,L)}{N} \quad &\geq \quad 4\pi\mu a\rho\Big(1 - (const.)Y^{-1}(a/l)^3\Big) \\ &\times \quad \Big(1 - \frac{l^3}{(R^3 - R_0^3)}\frac{const.Y}{\varepsilon(a/l)^2 - const.Y^2(l/a)^3}\Big). \end{aligned} \tag{2.84}$$

We are ultimately ready to make the ansatz

$$\varepsilon \sim Y^\alpha \qquad a/l \sim Y^\beta \qquad (R^3 - R_0^3)/l^3 \sim Y^\gamma. \tag{2.85}$$

The conditions on α, β, γ are:

- $\varepsilon(a/l)^2 - const.Y^2(l/a)^3 > 0$: holds for Y small enough, whenever $\alpha + 5\beta < 2$.
- $\alpha > 0$, in order $\varepsilon \to 0$ for $Y \to 0$.
- $3\beta - 1 > 0$ in order that $Y^{-1}(l/a)^3 \to 0$ for $Y \to 0$.
- $1 - 3\beta + \gamma > 0$ in order that $Y(l/a)^3(R^3 - R_0^3)/l^3 \to 0$ for $Y \to 0$.
- $1 - \alpha - 2\beta - \gamma > 0$ to control the last factor in (2.84).

These are all met by taking $\alpha = 1/17$, $\beta = 6/17$ and $\gamma = 3/17$ as is shown in [13]. Moreover, $2R/l \sim Y^{\gamma/3} = Y^{1/17}$ up to higher order. The physical meaning of the exponents can be interpreted as the following relations:

$$a \ll R \ll \rho^{-1/3} \ll l \ll (\rho a)^{-1/2} \tag{2.86}$$

Thus, we can finally take the thermodynamic limit and hence the proof of theorems (2.4) and (2.5) has been completed.

An extension to a case, where the potential v does not have a finite range, but still has finite scattering length, is obtained by approximation by finite-range (i.e. compactly supported) potentials and controlling the change of the scattering length as $R_0 \to \infty$.

Chapter 3

Bose-Einstein Condensation and the Gross-Pitaevskii Theory

3.1 Trapped Bosons

The picture of a homogeneous dilute Bose gas, as discussed in chapter 2 is, however, not directly applicable to modern experiments, since the density of the gas at low temperatures is essentially taken to be uniform. Hence, our previous analysis does not reflect the true state of affairs in the laboratory. As a matter of fact, recent experiments use an additional trapping potential to confine the bosons breaking down the homogeneity of the density. Here, we model the trap by a slowly varying external potential, $V(x)$, which has the property that for large distances, $|\mathbf{x}| \to \infty$, $V(\mathbf{x}) \to \infty$. The new Hamiltonian of the system then reads:

$$H = \sum_{i=1}^{N} \{-\mu\Delta_i + V(\mathbf{x}_i)\} + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|) \tag{3.1}$$

We can always take for granted (by shifting the energy scale) that its ground state energy is 0, since energy, as a specific number, does not make any sense, but only energy difference does. Thus, we assume $V \geq 0$.

Very often in experiments the trapping potential is assumed to be harmonic. Then the natural energy scale for the problem is determined by the ground state and hence the relevant length scale turns out to be $\sqrt{\frac{\hbar}{m\omega}} = \sqrt{\frac{2\mu}{\hbar\omega}} := L_{osc}$, ω being the frequency, and is interpreted as a measure for the trap dimensions. For simplicity, one could normalise $L_{osc} = 1$ and use it as a unit length in this problem. Then the typical energy scale reads $\hbar\omega = 2\mu L_{osc}^{-2} = 2\mu$.

Throughout this section we shall be dealing with a rigorous proof of the ground state energy for the above Hamiltonian in a scaling limit, called the Gross-Pitaevskii limit. We shall, of course, make use of our results for the energy of a dilute Bose gas in a finite box, obtained in chapter 2.

The limit we are interested in is $a \to 0$ while $N \to \infty$ with $Na = \text{const}$. This means that the interactions take place on a very small scale compared to the mean particle density. We therefore write the interaction potential as $v(|\mathbf{x}|) = a^{-2}v_1(|\mathbf{x}|/a)$. This allows us to vary a, while v_1 is a potential of unit scattering length. This relation is motivated by scaling of the zero energy scattering equation (2.4) by $\mathbf{x} \to a\mathbf{x}$, which together with (2.5) yields a unit scattering length for v_1. The reason we need to rescale the potential energy can be understood as follows: letting $N \to \infty$ in (3.1), one can easily convince oneself that the kinetic energy scales like N, while the potential energy goes like N^2. Hence, the interaction term would dominate over the kinetic one, violating the conditions of any experiment. Because of extensivity of the energy, both terms have to scale like N. The above rescaling of the interaction potential can be understood mathematically as increasing the strength of the interaction, but simultaneously decreasing its effective lengthscale. Therefore, in the limit $N \to \infty$, $Na = \text{const.}$, the interaction becomes effectively of the type $\frac{1}{N}\delta(\mathbf{x})$, when seen from a distributional point of view, and the $1/N$ correction suffices to restore the balance between the kinetic and potential terms. If we consider V and v_1 to be fixed, the ground state energy becomes a function of a and N, denoted as $E_0(a, N)$. It happens to posses a very specific scaling property discussed below.

The quantum mechanical ground state of (3.1) is the infimum of a functional, called the Gross-Pitaevskii (GP) functional. It arises physically in the following way: if we assume that the Bose gas is sufficiently dilute (i.e. for a very small), we write the corresponding wave function of the system, using a Hartree-Fock ansatz, as a product of a single-particle wave functions. It is well-known that this cannot be the general case, but this approximation turns out to be sufficient for our purposes.

$$\Psi(\mathbf{x}_1, ..., \mathbf{x}_N) = \prod_{i=1}^{N} \phi(\mathbf{x}_i) \tag{3.2}$$

If we further idealise by taking the interacting potential to be of δ-function type, given by $a^{-2}v_1(|\mathbf{x}_i - \mathbf{x}_j|/a) = 8\pi\mu a^{-2}\delta(|\mathbf{x}_i - \mathbf{x}_j|/a)$, and consider only radial trapping potentials, then the energy of the system is given by:

$$\begin{aligned} \mathcal{E}^{GP}[\Psi] &= \sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} \{\mu|\nabla_i \Psi|^2 + V(|\mathbf{x}_i|)|\Psi|^2 + \frac{1}{2} 8\pi\mu \sum_{j=1,\ j\neq i}^{N} a^{-2}\delta(|\mathbf{x}_i - \mathbf{x}_j|/a)|\Psi|^2\} \\ &= \int_{\mathbb{R}^3} N\mu|\nabla\phi|^2 + NV(|\mathbf{x}|)|\phi|^2 + 4\pi\mu a N(N-1)|\phi|^4 \end{aligned} \tag{3.3}$$

where we used the symmetry of the bosonic wave function as well as its normatisation $\int |\Psi|^2 = 1$. In the 3D case of a single particle, normalised according to $\int |\phi|^2 = N$, we therefore have:

$$\mathcal{E}^{GP}[\phi] = \int_{\mathbb{R}^3} \mu|\nabla\phi|^2 + V|\phi|^2 + 4\pi\mu a|\phi|^4 \tag{3.4}$$

The ground state energy is attained by the minimiser of the above functional, denoted ϕ^{GP}[1], depending on N and a , and has the following properties:

Lemma 3.1. *The GP functional has a unique (up to a phase factor) minimiser, satisfying:*

- ϕ^{GP} *is at least once continuously differentiable and if* $V \in C^\infty$*, then also* $\phi^{GP} \in C^\infty$*.*
- *The irrelevant phase factor can be chosen such that* $\phi^{GP} > 0$*.*
- *The ground state energy* $E^{GP}(N, a)$ *is continuously differentiable in* a*, and (by the scaling relation discussed below) also in* N*.*

[1] whenever this dependence is important we shall denote it by $\phi^{GP}_{a,N}$

- *The minimiser ϕ^{GP} solves the GP-equation*

$$-\Delta\phi + V\phi + 8\pi a|\phi|^2\phi = \mu\phi \tag{3.5}$$

where $\mu = \mathrm{d}E^{GP}(a,N)/\mathrm{d}N = E^{GP}(a,N)/N + (4\pi\mu a/N)\int|\phi^{GP}|^4$ is the chemical potential.

- *If V is spherically symmetric and monotone increasing, then ϕ^{GP} is spherically symmetric and monotone decreasing.*

- *If V is convex, then ϕ^{GP} is* log-concave*, i.e. $\phi^{GP}(\boldsymbol{x})^\lambda\phi^{GP}(\boldsymbol{y})^{1-\lambda} \leq \phi^{GP}(\lambda\boldsymbol{x} + (1-\lambda)\boldsymbol{y})$ for all $\boldsymbol{x}$,$\boldsymbol{y} \in \mathbb{R}^3$ and $\lambda \in (-1,1)$*

- *For all $t > 0$ there exists a constant M_t, such that $\phi^{GP} \leq M_t e^{-t|\boldsymbol{x}|}$. In particular, $\phi^{GP} \in L^\infty$ decreases faster than exponentially at infinity.*

Proof. The proof of the Lemma can be found in Appendix A of [14]. □

Thus, for the ground state energy in the GP limit we have:

$$E^{GP}(N,a) = \mathcal{E}^{GP}[\phi^{GP}]. \tag{3.6}$$

The GP theory has the following scaling properties:

$$E^{GP}(N,a) = NE^{GP}(1,aN) \tag{3.7}$$
$$\phi^{GP}_{a,N} = N^{1/2}\phi^{GP}_{1,aN}, \tag{3.8}$$

whence we infer that the important parameter will be the product Na. They are easily obtained from the definition of the ground state energy.

We also see that, for $V(\mathbf{x}) = 0$ inside a large box of side length L, and ∞ otherwise, $\phi^{GP} \approx \sqrt{N/L^3}$ and we obtain the well-established relation $E^{GP} = 4\pi\mu aN^2/L^3$ for the homogeneous dilute Bose gas.

However, here we are interested in a limit, where all three terms in the Hamiltonian (3.1) make a contribution. Fixing Na as $N \to \infty$ will be referred to as the 'GP limit'. In this case we shall prove that

$$E_0 \approx E^{GP} \text{ and } \rho^{QM}(\mathbf{x}) \approx |\phi^{GP}(\mathbf{x})|^2 := \rho^{GP}(\mathbf{x}), \tag{3.9}$$

with the quantum mechanical particle density in the ground state defined as

$$\rho^{QM}(\mathbf{x}) := N\int|\Psi(\mathbf{x},\mathbf{x}_2,...,\mathbf{x}_N)|\mathrm{d}\mathbf{x}_2...\mathrm{d}\mathbf{x}_N. \tag{3.10}$$

In order to make use of the results established in the previous chapter we consider a low density regime, defined as $\bar{\rho}a^3 \ll 1$, where

$$\bar{\rho} = \frac{1}{N}\int|\rho^{GP}(\mathbf{x})|^2\mathrm{d}\mathbf{x} \tag{3.11}$$

is the mean particle density. Consequently, fixing Na actually means that the GP limit is a dilute limit, because $\bar{\rho}_{N,a} = N\bar{\rho}_{1,Na}$ and thus $\bar{\rho} \sim N$ and $\bar{\rho}a^3 \sim N^{-2}$. The following theorem makes out of our analysis a rigorous statement:

Theorem 3.2. ***(GP limit of the QM ground state energy and density).*** *In the GP limit, i.e. for $N \to \infty$ with Na held fixed, we have*

$$\lim_{N\to\infty} \frac{E_0^{QM}(N,a)}{E^{GP}(N,a)} = 1, \tag{3.12}$$

and

$$\lim_{N\to\infty} \frac{1}{N} \rho_{N,a}^{QM}(\boldsymbol{x}) = |\phi_{1,Na}^{GP}(\boldsymbol{x})|^2 \tag{3.13}$$

in the weak L^1-sense.

Given the convergence of the energies (3.12), the convergence of the densities (3.13) is proved by variation of the external potential. Define the variation of V as

$$V(\mathbf{x}) \longrightarrow V(\mathbf{x}) + \delta Z(\mathbf{x}) \tag{3.14}$$

for some positive $Z \in C_0^\infty$. Following exactly the same procedure as given below, one could prove the upper and lower bounds for the new potential. Differentiation with respect to δ and evaluating at $\delta = 0$ finally yields

$$\lim_{N\to\infty} \frac{1}{N} \rho_{N,a}^{QM}(\mathbf{x}) = |\phi_{1,Na}^{GP}(\mathbf{x})|^2 \tag{3.15}$$

in the sense of distributions (notice that $\langle \Psi, Z\Psi \rangle = \int \rho^{QM} Z$ for any $Z \in C_0^\infty$). Since $\phi_{1,Na}^{GP}(\mathbf{x})$ decreases faster than exponentially at infinity, while $\rho_{N,a}^{QM}(\mathbf{x})$ has finite L^1-norm (wave functions are elements of L^2), we infer L^1-weak convergence by a standard approximation argument.

The proof of the statement (3.12) is worked out in the subsequent two sections.

3.2 Upper Bound

An upper bound on the ground state energy can be obtained in the very same way as for the dilute case of uniform density in a finite box. However, a slight modification of the trial wave function is needed, to take into account the external trapping potential. For simplicity, we set $\mu = 1$.

Theorem 3.3 (Upper Bound)**.** *For $a\bar{\rho}^{1/3}$ small enough the following upper bound on the quantum mechanical ground state energy in the GP limit holds:*

$$E_0^{QM}(N,a) \leq E^{GP}(N,a)(1 + O(a\bar{\rho}^{1/3})). \tag{3.16}$$

Proof. Since the bosonic ground state energy, i.e. the infimum of the quadratic form taken over all symmetric wave functions, is the same as the absolute ground state energy, i.e. the infimum taken over the whole tensor product space $L^2(\mathbb{R}^{3N})$, it suffices to construct a trial state neglecting the symmetry condition, provided it catches the essence of the bosonic interparticle interaction. Given the minimiser ϕ^{GP}, we set

$$\Psi(\mathbf{x}_1, ..., \mathbf{x}_N) = F(\mathbf{x}_1, ..., \mathbf{x}_N) G(\mathbf{x}_1, ..., \mathbf{x}_N), \tag{3.17}$$

where

$$F(\mathbf{x}_1, ..., \mathbf{x}_N) = \prod_{i=1}^{N} F_i(\mathbf{x}_1, ..., \mathbf{x}_N) \tag{3.18}$$

are defined precisely the same way as in Senction 2.2 and

$$G(\mathbf{x}_1, ..., \mathbf{x}_N) = \prod_{i=1}^{N} \frac{\phi^{GP}(\mathbf{x}_i)}{||\phi^{GP}||_\infty}. \tag{3.19}$$

Let us in the following denote

$$g(\mathbf{x}) = \frac{\phi^{GP}(\mathbf{x})}{||\phi^{GP}||_\infty}. \tag{3.20}$$

The idea behind this particular choice is similar to the one used in Section 2.2. Particles are being inserted into the system one by one, without adjusting their wave functions to the ones of the already present particles. The modification $g(\mathbf{x})$ should capture the additional Gross-Pitaevskii terms allowing for an upper bound of the current theorem. It should be mentioned here that this type of trial function is not believed to represent the true state of affairs, since it does not account for inter-particle correlations.
In the following, we aim at estimating the normalised ground state energy $\langle \Psi | H \Psi \rangle / \langle \Psi | \Psi \rangle$ from above. The kinetic term can be recast as

$$\int_{\mathbb{R}^{3N}} \Psi \nabla_k^2 \Psi = \int_{\mathbb{R}^{3N}} (G \nabla_k^2 G) F^2 - \int_{\mathbb{R}^{3N}} G^2 |\nabla_k F|^2 \tag{3.21}$$

where the subindex k denotes the derivative with respect to the k^{th} variable. Using definitions (3.18) and (3.19), we obtain in a very similar fashion as in (2.22)

$$G \nabla_k F = \sum_{i=1}^{N} \Psi F_i^{-1} \varepsilon_{ik} n_i f'(t_i). \tag{3.22}$$

Next, we sum up over k to obtain

$$\begin{aligned} |\Psi|^{-2} \sum_k G^2 |\nabla_k \Psi|^2 &= \sum_{i,k,j} \varepsilon_{ik} \varepsilon_{jk} \mathbf{n}_i \cdot \mathbf{n}_j F_i^{-1} F_j^{-1} f'(t_i) f'(t_j) \\ &\leq 2 \sum_{k \leq i < j} |\varepsilon_{ik} \varepsilon_{jk}| F_i^{-1} F_j^{-1} f'(t_i) f'(t_j) + 2 \sum_i F_i^{-2} f'^2(t_i). \end{aligned} \tag{3.23}$$

Notice that all the contribution from G is cancelled by the prefactor $|\Psi|^{-2}$. Let us now consider the normalised quadratic form of the energy functional:

$$\begin{aligned} \frac{\langle \Psi, H_N \Psi \rangle}{\langle \Psi, \Psi \rangle} \leq & \underbrace{2 \sum_{i=1}^{N} \frac{\int |\Psi|^2 F_i^{-2} f'^2(t_i)}{\int |\Psi|^2} + \sum_{1 \leq j < i \leq N} \frac{\int |\Psi|^2 v(|\mathbf{x}_i - \mathbf{x}_j)}{\int |\Psi|^2}}_{=J_1} \\ & + \underbrace{2 \sum_{k \leq i < j} \frac{\int |\Psi|^2 |\varepsilon_{ik} \varepsilon_{jk}| F_i^{-1} F_j^{-1} f'(t_i) f'(t_j)}{\int |\Psi|^2}}_{=J_2} \\ & + \underbrace{\sum_{i=1}^{N} \frac{\int |\Psi|^2 \{-g(\mathbf{x}_i)^{-1} \nabla_i^2 g(\mathbf{x}_i) + V(\mathbf{x}_i)\}}{\int |\Psi|^2}}_{=J_3} \end{aligned} \tag{3.24}$$

Recall the definition of $F_{p,i}$ and $F_{p,ij}$ from Section 2.2 as well as inequalities (2.29), (2.31) and (2.32). The way they will be used in the current proof is exactly the same as in Section 2.2. Our goal shall again be to estimate the $\mathbf{x}_i$ and $\mathbf{x}_j$ integrals in the numerators and the denominators. The only difference this time comes from the presence of g. To this end, define the following transformation:

$$\begin{aligned} \eta &:= \mathbf{x}_i - \mathbf{x}_j \\ \chi &:= \frac{\mathbf{x}_i + \mathbf{x}_j}{2} \end{aligned} \tag{3.25}$$

Then we obtain

$$\begin{aligned} &\int \{2f'^2(|\mathbf{x}_i - \mathbf{x}_j|) + v(|\mathbf{x}_i - \mathbf{x}_j|)f^2(|\mathbf{x}_i - \mathbf{x}_j|)\} g(\mathbf{x}_i)^2 g(\mathbf{x}_j)^2 \mathrm{d}\mathbf{x}_i \mathrm{d}\mathbf{x}_j \\ &\qquad = \int \{2f'^2(|\eta|) + v(|\eta|)f^2(|\eta|)\} g(\chi + \frac{1}{2}\eta)^2 g(\chi - \frac{1}{2}\eta)^2 \mathrm{d}\eta \mathrm{d}\chi. \end{aligned} \tag{3.26}$$

By the Schwarz inequality one gets

$$\int g(\chi + \frac{1}{2}\eta)^2 g(\chi - \frac{1}{2}\eta)^2 \mathrm{d}\chi \leq \int g(\chi)^4 \mathrm{d}\chi \tag{3.27}$$

and hence

$$\begin{aligned} &\int \{2f'^2(|\mathbf{x}_i - \mathbf{x}_j|) + v(|\mathbf{x}_i - \mathbf{x}_j|)f^2(|\mathbf{x}_i - \mathbf{x}_j|)\} g(\mathbf{x}_i)^2 g(\mathbf{x}_j)^2 \mathrm{d}\mathbf{x}_i \mathrm{d}\mathbf{x}_j \\ \leq &\int g(\chi)^4 \mathrm{d}\chi \int 2f'^2(|\eta|) + v(|\eta|)f^2(|\eta|)\mathrm{d}\eta \overset{(2.33)}{=} 8\pi a(1 - a/b)^{-1} \int g(\chi)^4 \mathrm{d}\chi. \end{aligned} \tag{3.28}$$

The analogue of (2.35) then clearly reads

$$\begin{aligned} \int \left[1 - \sum_{k=1; k\neq i}^{N} \{(1 - f^2(|\mathbf{x}_i - \mathbf{x}_k|))\} g(\mathbf{x}_i)^2 \right] \mathrm{d}\mathbf{x}_i \quad &\geq \\ \int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - (N-1) \int (1 - f^2(|\mathbf{x}_i - \mathbf{x}_k|)) \quad &\geq \quad \int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI \end{aligned} \tag{3.29}$$

where I is defined in (2.35).

Inserting the above results into (3.24) and following the same strategy as in Section 2.2 we see that the first and the second terms (i.e. the expression denoted by J_1) are bounded from above by

$$\sum_{i=1}^{N} (i-1) \frac{8\pi a(1 - a/b)^{-1} \int g(\chi)^4 \mathrm{d}\chi}{\left(\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI\right)^2} \leq N^2 \frac{4\pi a(1 - a/b)^{-1} \int g(\chi)^4 \mathrm{d}\chi}{\left(\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI\right)^2}. \tag{3.30}$$

In the third term in (3.24), J_3, we note that the summation is effectively taken over two distinct values of k only. Moreover, $k = i$ will definitely be non-zero by definition of ε_{ik} and hence the two equal contributions come from $k = i$ and $k < i$. Then, we can estimate

$$
\begin{aligned}
&\sum_{k=1}^{i} \int |\varepsilon_{ik}\varepsilon_{jk}| f(t_i) f(t_j) f'(t_i) f'(t_j) g(\mathbf{x}_i)^2 g(\mathbf{x}_j)^2 \mathrm{d}\mathbf{x}_i \mathrm{d}\mathbf{x}_j \\
\leq\ & 2\sum_{k=1}^{i-1} f(|\mathbf{x}_i - \mathbf{x}_k|) f(\mathbf{x}_j - \mathbf{x}_k|) f'(|\mathbf{x}_i - \mathbf{x}_k|) f'(|\mathbf{x}_j - \mathbf{x}_k|) g(\mathbf{x}_i)^2 g(\mathbf{x}_j)^2 \mathrm{d}\mathbf{x}_i \mathrm{d}\mathbf{x}_j \\
&\stackrel{g\leq 1}{\leq} 2\sum_{k=1}^{i-1} f(|\mathbf{x}_i|) f(\mathbf{x}_j|) f'(|\mathbf{x}_i|) f'(|\mathbf{x}_j|) \mathrm{d}\mathbf{x}_i \mathrm{d}\mathbf{x}_j \\
&= 2(i-1)\Big(\int f(|\mathbf{x}|) f'(|\mathbf{x}|) \mathrm{d}\mathbf{x} \Big)^2 = 2(i-1)K^2
\end{aligned}
\tag{3.31}
$$

where K is defined via (2.42). Exactly as before, summing over i and j yields a factor of $\frac{1}{6}N(N-1)(N-2)$. Taking into account the contribution from the denominator, we finally obtain the following bound for J_2:

$$
\frac{2}{3} \frac{N^3 K^2}{\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI}.
\tag{3.32}
$$

Now, consider the last and most important term J_3. Notice that it's appearance is exclusively due to the GP minimizer present via g and, therefore, does not occur in our previous discussion in Section 2.2. Define a number $\tilde{e} \in \mathbb{R}$ by

$$
\int -g(\mathbf{x}) \nabla^2 g(\mathbf{x}) + V(\mathbf{x}) g(\mathbf{x})^2 \mathrm{d}\mathbf{x} =: \tilde{e} \int g(\mathbf{x})^2 \mathrm{d}\mathbf{x}
\tag{3.33}
$$

Then, using that $F \leq 1$ and writing out the factor $|\Psi|^2$, we obtain

$$
\begin{aligned}
&\sum_{i=1}^{N} \frac{\int_{\mathbb{R}^{3N}} |\Psi|^2 \{-g(\mathbf{x}_i)^{-1} \nabla_i^2 g(\mathbf{x}_i) + V(\mathbf{x}_i)\}}{\int_{\mathbb{R}^{3N}} |\Psi|^2} \\
= &\sum_{i=1}^{N} \frac{\int_{\mathbb{R}^{3N}} \prod_{m=1}^{N} g(\mathbf{x}_m^2) F_m^2 \{-g(\mathbf{x}_i)^{-1} \nabla_i^2 g(\mathbf{x}_i) + V(\mathbf{x}_i)\}}{\int_{\mathbb{R}^{3N}} |\Psi|^2} \\
\stackrel{F_i\leq 1}{\leq} &\sum_{i=1}^{N} \frac{\int_{\mathbb{R}} |\nabla g(\mathbf{x})|^2 + V(\mathbf{x}) g(\mathbf{x})^2}{\int_{\mathbb{R}} g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI} \leq \frac{N\tilde{e} \int g(\mathbf{x})^2 \mathrm{d}\mathbf{x}}{\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI}.
\end{aligned}
\tag{3.34}
$$

Altogether, this yields

$$
\begin{aligned}
\frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle} \leq N \frac{\tilde{e} \int g(\mathbf{x})^2 \mathrm{d}\mathbf{x}}{\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI} &+ N^2 \frac{4\pi a (1 - a/b)^{-1} \int g(\mathbf{x})^4 \mathrm{d}\mathbf{x}}{\big(\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI \big)^2} \\
&+ \frac{2}{3} N^3 \frac{K^2}{\big(\int g(\mathbf{x})^2 \mathrm{d}\mathbf{x} - NI \big)^2}.
\end{aligned}
\tag{3.35}
$$

In Section 2.2 the following bounds on K and I have been proved:

$$
\begin{aligned}
I &\leq \frac{4\pi}{3} a b^2 \\
K &\leq 4\pi a b \big(1 + O(a/b) \big)
\end{aligned}
\tag{3.36}
$$

with the corresponding definitions of a and b.

We now have to estimate the g-integrals further. Recall the definition of the mean density $\bar{\rho}$:

$$\bar{\rho} = \frac{1}{N}\int (\rho^{GP})^2 = N\frac{\int g^4}{\left(\int g^2\right)^2} \tag{3.37}$$

where the last equality is owing to $\int \rho^{GP} = N$. Consequently, we can choose the free parameter b by

$$\frac{4\pi}{3}\bar{\rho}b^3 = \frac{\int g^4}{\int g^2} = \frac{\bar{\rho}}{||\rho^{GP}||_\infty} =: c. \tag{3.38}$$

Then the denominator occurring ubiquitously in (3.35), using the relations we have just obtained, is bounded from below by

$$\int g^2 - NI = \int g^2(1-\frac{NI}{\int g^2}) = \int g^2(1-\frac{3NI}{4\pi N b^3}) \geq \int g^2(1-\frac{3\times 4\pi a b^2}{4\pi 3 b^3}) = (1-a/b)\int g^2. \tag{3.39}$$

We remark that $c \leq 1$, and $a < b$ holds provided

$$\frac{a^3}{b^3} = \frac{4\pi}{3}a^3||\rho^{GP}||_\infty < 1. \tag{3.40}$$

Let us now complete the estimates on the three integrals in (3.35). For the first one we have

$$\begin{aligned} N\frac{\tilde{e}\int g(\mathbf{x})^2\mathrm{d}\mathbf{x}}{\int g(\mathbf{x})^2\mathrm{d}\mathbf{x} - NI} &\leq N\frac{\tilde{e}\int g^2}{(1-a/b)\int g^2} = N\tilde{e}(1+O(a/b)) \\ &= N\frac{\int |\nabla g|^2 + Vg^2}{\int g^2}(1+O(a/b)) \\ &= \frac{N}{||\phi^{GP}||_2^2}\frac{||\phi^{GP}||_\infty^2 \int |\nabla\phi^{GP}|^2 + V|\phi^{GP}|^2}{||\phi^{GP}||_\infty^2}(1+O(a/b)) \\ &= \int |\nabla\phi^{GP}|^2 + V|\phi^{GP}|^2(1+O(a/b)). \end{aligned} \tag{3.41}$$

Similarly, the second one is estimated from above by

$$\begin{aligned} N^2\frac{4\pi a(1-a/b)^{-1}\int g(\mathbf{x})^4\mathrm{d}x}{\left(\int g(\mathbf{x})^2\mathrm{d}\mathbf{x} - NI\right)^2} &\leq N^2\frac{4\pi a}{(1-a/b)^3}\frac{\int g^4}{(\int g^2)^2} \\ &= 4\pi a\frac{N^2}{(\int |\phi^{GP}|^2)^2}\int |\phi^{GP}|^4(1+O(a/b)) \\ &= 4\pi a\frac{||\phi^{GP}||_\infty^4}{(\int |\phi^{GP}|^2)^2}\int |\rho^{GP}|^2(1+O(a/b)) \\ &= 4\pi a\int |\rho^{GP}|^2(1+O(a/b)). \end{aligned} \tag{3.42}$$

For the last integral, we obtain

$$\begin{aligned}
\frac{2}{3}N^3\frac{K^2}{\left(\int g(\mathbf{x})^2\mathrm{d}\mathbf{x}-NI\right)^2} &\leq \frac{2}{3}\frac{N^2K^2}{(1-a/b)^2(\int g^2)^2} \leq \frac{2}{3}\frac{N^2 4\pi 4\pi a^2 b^2}{(\int g^2)^2}(1+O(a/b)) \\
&= 4\pi a\frac{2a}{b}\frac{4\pi b^3}{3}N^3\frac{||\phi^{GP}||_\infty^4}{(\int|\phi^{GP}|^2)^2}(1+O(a/b)) \\
&\overset{N=\frac{\int|\rho^{GP}|^2}{\bar\rho}}{=} 4\pi a\frac{2a}{b}\frac{4\pi b^3}{3}\frac{\int|\rho^{GP}|^2}{\bar\rho}||\phi^{GP}||_\infty^4(1+O(a/b)) \\
&\overset{\frac{4\pi}{3}b^3=1/||\rho^{GP}||_\infty}{=} 4\pi a\frac{2a}{b}\frac{||\phi^{GP}||_\infty^2}{\bar\rho}\frac{||\phi^{GP}||_\infty^2}{||\rho^{GP}||_\infty}\int|\rho^{GP}|^2(1+O(a/b)) \\
&\overset{||\phi^{GP}||_\infty^2/\bar\rho=1/c}{=} 4\pi a\frac{2}{c}\int|\rho^{GP}|^2 O(a/b). \qquad (3.43)
\end{aligned}$$

Putting these estimates together finally proves the theorem. □

3.3 Lower Bound

The lower bound is more complicated to obtain and will be given in full detail. We make use of the 'cell method' again dividing the space into boxes of finite size. The goal shall be to apply the well-established bound (2.84) to these cells with Neumann boundary conditions, keeping the energy as low as possible. Neglecting the interaction between neighbouring boxes can only decrease the energy of the system (notice again that v is positive, so we can just drop the relevant terms where appropriate). Finally, we minimise over all possible distributions of particles to arrive at the final estimate.

Theorem 3.4. *The ground state energy of a trapped dilute bose gas, for Na held fixed is bouded from below as follows:*

$$\liminf_{N\to\infty}\frac{E_0^{QM}(N,a)}{E^{GP}(N,a)} \geq 1. \qquad (3.44)$$

Proof. We begin by factoring out the GP wave function from the total one. Since ϕ^{GP} is strictly positive, equation (3.17) determines F. Notice that Ψ is not necessarily normalised. We proceed further by computing the expectation value of the Hamiltonian (3.1) in this state:

$$\begin{aligned}
\langle\Psi, H\Psi\rangle &= \sum_{i=1}^N\int|\Psi|^2\phi^{GP}(\mathbf{x}_i)^{-1}[-\nabla_i^2+V(\mathbf{x}_i)]\phi^{GP}(\mathbf{x}_i)+ \\
&+ \prod_{k=1}^N\phi^{GP}(\mathbf{x}_k)|\nabla_i F|^2+\frac{1}{2}\sum_{j=1}^N\sum_{j\neq i}|\Psi|^2 v(|\mathbf{x}_i-\mathbf{x}_j|), \qquad (3.45)
\end{aligned}$$

where we made use of the fact that

$$\nabla_i\Psi=\nabla_i\Big(F\prod_k\phi_k\Big)=(\nabla_i F)\prod_k\phi_k+F\prod_k\phi_k\frac{\nabla_i\Big(F\prod_k\phi_k\Big)}{\prod_k\phi_k}=\Psi\frac{\nabla_i\phi_i}{\phi_i}. \qquad (3.46)$$

Inserting the GP equation,

$$\langle \Psi, H\Psi \rangle = \sum_{i=1}^{N} \int \prod_{k=1}^{N} \rho^{GP}(\mathbf{x}_k) \Big[|\nabla_i F|^2 + (\mu - 8\pi a \rho^{GP} + \frac{1}{2} \sum_{j=1\ j\neq i}^{N} v(|\mathbf{x}_i - \mathbf{x}_j|))|F|^2 \Big], \quad (3.47)$$

and the definition of μ we arrive at

$$E_0(N,a) - E^{GP}(N,a) \geq 4\pi a \int |\rho^{GP}|^2 + Q(F), \quad (3.48)$$

where the quadratic form $Q(F)$ is given by:

$$Q(F) := \inf_{\int |\Psi|^2 = 1} \sum_{i=1}^{N} \frac{\int \prod_{k=1}^{N} \rho^{GP}(\mathbf{x}_k) \Big[|\nabla_i F|^2 - 8\pi a \rho^{GP}(\mathbf{x}_i) + \frac{1}{2} \sum_{j=1\ j\neq i}^{N} v(|\mathbf{x}_i - \mathbf{x}_j|)|F|^2 \Big]}{\int \prod_{k=1}^{N} \rho^{GP}(\mathbf{x}_k)|F|^2}. \quad (3.49)$$

Clearly, we have to minimise Q in a suitable way. Comparison to the energy of Ψ yields:

$$V(\mathbf{x}) \longrightarrow -8\pi a \rho^{GP}(\mathbf{x}) \quad \text{and} \quad \prod_{k=1}^{N} \mathrm{d}\mathbf{x}_k \longrightarrow \prod_{k=1}^{N} \rho^{GP}(\mathbf{x}_k)\mathrm{d}\mathbf{x}_k \quad (3.50)$$

which implies a correct measure for this problem.

Next, we divide space into cells, as mentioned above, labelled by α. By Q_α we denote the quadratic form with integration restricted to the box α containing n_α particles. By doing so, we obtain the natural constraint $\sum_\alpha n_\alpha = N$ and clearly

$$\inf_F Q(F) \geq \inf_{\{n_\alpha\}} \sum_\alpha \inf_{F_\alpha} Q_\alpha(F_\alpha) \quad (3.51)$$

takes this into account as well.

We proceed by fixing a number $M > 0$ (cf. the properties of the GP minimiser), and focus our attention on the cells inside a big box Λ_M of side length M. Dropping the interaction between contiguous cells, as discussed at the beginning of the proof, lowers the energy. The contribution of (3.49) outside Λ_M is estimated as follows: consider the quadratic form, with integration restricted outside Λ_M this time. Dropping the v and ∇_i terms goes further in the good direction. But then we can estimate ρ^{GP} by its supremum, take it out of the integral, cancelling the numerator and the denominator. Summing up over the free index i picks up a factor of N which, taken back under the supremum and using the scaling relation (3.8) and the definition of $\rho^{GP}(\mathbf{x})$, (3.9), gives the lower bound $-8\pi a \sup_{\mathbf{x}\notin\Lambda_M} |\phi^{GP}_{1,Na}(\mathbf{x})|^2$. Recalling that the minimiser decreases faster than exponentially at infinity shows that the contribution of $Q(F)$ outside the big box tends to 0 as $M \to \infty$.

Inside each cell α the idea is now to approximate the density by constants from both below and above, for optimal control. Let us therefore denote by $\rho_{\alpha,max}$ and $\rho_{\alpha,min}$ its maximal and minimal value, respectively. Notice that since the minimiser is continuous and the cells compact sets, both of these values exist. Define

$$\Psi_\alpha(\mathbf{x}_1, ..., \mathbf{x}_{n_\alpha}) := F_\alpha(\mathbf{x}_1, ..., \mathbf{x}_{n_\alpha}) \prod_{k=1}^{n_\alpha} \phi^{GP}(\mathbf{x}_k), \quad (3.52)$$

and

$$\Psi_\alpha^i(\mathbf{x}_1, ..., \mathbf{x}_{n_\alpha}) := F_\alpha(\mathbf{x}_1, ..., \mathbf{x}_{n_\alpha}) \prod_{k=1,\ k\neq i}^{n_\alpha} \phi^{GP}(\mathbf{x}_k). \tag{3.53}$$

Then, for all $1 \leq i \leq n_\alpha$:

$$\begin{aligned} &\int \prod_{k=1}^{n_\alpha} \rho^{GP}(\mathbf{x}_k) \left(|\nabla_i F_\alpha|^2 + \frac{1}{2} \sum_{j=1,\ j\neq i}^{N} v(|\mathbf{x}_i - \mathbf{x}_j|)|F_\alpha|^2 \right) \\ &\geq \rho_{\alpha,min} \int \left(|\nabla_i \Psi_\alpha^i|^2 + \frac{1}{2} \sum_{j=1,\ j\neq i}^{N} v(|\mathbf{x}_i - \mathbf{x}_j|)|\Psi_\alpha^i|^2 \right) \end{aligned} \tag{3.54}$$

where we use the above definitions and the fact that the product can be taken inside $|\nabla_i \cdot|$, whenever the index i is omitted and the integrand is positive.

Next, use Lemma 2.6 to trade kinetic for potential energy, resulting in

$$(3.54) \geq \rho_{\alpha,min} \int (\varepsilon|\nabla_i \Psi_\alpha^i|^2 + (1-\varepsilon)U(t_i)|\Psi_\alpha^i|^2) \tag{3.55}$$

with t_i the distance to the nearest neighbour of $\mathbf{x}_i$ and U the potential in (2.55).

Lemma 3.5. *For $E_\varepsilon^U(n_\alpha, L)$, the ground state energy of*

$$\tilde{H}_n = \sum_{i=1}^{n_\alpha} (-\frac{1}{2}\varepsilon\Delta_i + (1-\varepsilon)aU(t_i)), \tag{3.56}$$

and C_M given by

$$C_M = \frac{1}{N} \sup_{\boldsymbol{x}\in\Lambda_M} |\nabla_i \phi^{GP}(\boldsymbol{x}_i)|^2 = \sup_{\boldsymbol{x}\in\Lambda_M} |\nabla_i \phi^{GP}_{1,Na}(\boldsymbol{x}_i)|^2 \tag{3.57}$$

we have

$$Q_\alpha(F_\alpha) \geq \frac{\rho_{\alpha,min}}{\rho_{\alpha,max}} E_\varepsilon^U(n_\alpha, L) - 8\pi a \rho_{\alpha,max} n_\alpha - \varepsilon C_M n_\alpha. \tag{3.58}$$

Proof. Using the relation $\Psi_\alpha = \phi^{GP}(\mathbf{x}_i)\Psi_\alpha^i$, we get

$$\begin{aligned} |\nabla_i \Psi_\alpha|^2 &= |\nabla_i \phi^{GP}(\mathbf{x}_i)\Psi_\alpha^i|^2 \\ &= |(\nabla_i \phi^{GP}(\mathbf{x}_i))\Psi_\alpha^i + \phi^{GP}(\mathbf{x}_i)\nabla_i \Psi_\alpha^i|^2 \\ &\leq 2(|\underbrace{(\nabla_i \phi^{GP}(\mathbf{x}_i))}_{\leq \sup_{\mathbf{x}\in\Lambda_M} |\nabla_i \phi^{GP}(\mathbf{x}_i)|} \Psi_\alpha^i|^2 + |\underbrace{\phi^{GP}(\mathbf{x}_i)}_{\leq \rho_{\alpha,max}} \nabla_i \Psi_\alpha^i|^2) \\ &\leq 2C_M N|\Psi_\alpha^i|^2 + 2\rho_{\alpha,max}|\nabla_i \Psi_\alpha^i|^2. \end{aligned} \tag{3.59}$$

independent of N in the GP limit. Next, we rewrite (3.59):

$$|\nabla_i \Psi_\alpha^i|^2 \geq \frac{|\nabla_i \Psi_\alpha|^2}{2\rho_{\alpha,max}} - \frac{C_M N |\Psi_\alpha^i|^2}{\rho_{\alpha,max}}, \tag{3.60}$$

plug it in (3.55) and sum over i up to n_α, obtaining

$$\sum_{i=1}^{n_\alpha} \rho_{\alpha,min} \int_{\Lambda_M} \frac{\varepsilon}{2\rho_{\alpha,max}} |\nabla_i \Psi_\alpha|^2 - \varepsilon \frac{C_M N |\Psi_\alpha^i|^2}{\rho_{\alpha,max}} + a(1-\varepsilon) \frac{U(t_i)}{\rho^{GP}(\mathbf{x}_i)} \underbrace{|\Psi_\alpha^i|^2 \rho^{GP}(\mathbf{x}_i)}_{=|\Psi_\alpha|^2}. \quad (3.61)$$

Then, using $\rho^{GP}(\mathbf{x}_i) \leq \rho_{\alpha,max}$ in the second term of the numerator of (3.49), after performing the summation and cancelling the remnants in the numerator and the denominator, we pick up a factor $-8\pi a \rho_{\alpha,max} n_\alpha$. We also have

$$\sum_{i=1}^{n_\alpha} \rho_{\alpha,min} \int_{\Lambda_M} \frac{C_M N |\Psi_\alpha^i|^2}{\rho_{\alpha,max}} \leq N C_M n_\alpha \int_{\Lambda_M} |\Psi_\alpha^i|^2 \quad (3.62)$$

In the denominator of (3.49), we use once again $\Psi_\alpha = \phi^{GP}(\mathbf{x}_i)\Psi_\alpha^i$, together with the normalization condition $\int \rho^{GP} = N$, to cancel the N. The remaining integrals in the numerator and the denominator also cancel. Therefore, we obtain for the normalized quadratic form Q

$$Q_\alpha(F_\alpha) \geq \frac{\rho_{\alpha,min}}{\rho_{\alpha,max}} E_\varepsilon^U(n_\alpha, L) - 8\pi a \rho_{\alpha,max} n_\alpha - \varepsilon C_M n_\alpha \quad (3.63)$$

completing the proof of the Proposition. □

The goal is now to minimise the resulting expression under the constraint $\sum_\alpha n_\alpha = N$. If we drop it, we enlarge the set the infimum is taken over, which lowers it once again. In the subsequent discussion the term $\varepsilon C_M n_\alpha$ shall not play any role, and will therefore be left out of consideration.

We now use our knowledge about a lower bound to the ground state energy of the operator (3.56), obtained in section 2.3:

$$E_\varepsilon^U(n_\alpha, L) \geq (1-\varepsilon) \frac{4\pi a n_\alpha^2}{L^3} (1 - C Y_\alpha^{1/17}) \quad (3.64)$$

with $Y_\alpha = a^3 n_\alpha / L^3$, provided Y_α is small enough, $\varepsilon \geq Y_\alpha^{1/17}$ and $n_\alpha \geq const. Y_\alpha^{-1/17}$. Choosing $\varepsilon = Y^{1/17}$ satisfies the second condition. The next thing to show is that the minimising n_α is large enough for the third condition still to be fulfilled.

Suppose the minimum in the RHS of (3.63) is taken for some $\bar{n}_\alpha$. Then, clearly

$$\frac{\rho_{\alpha,min}}{\rho_{\alpha,max}} (E_\varepsilon^U(\bar{n}_\alpha + 1, L) - E_\varepsilon^U(\bar{n}_\alpha, L)) \geq 8\pi a \rho_{\alpha,max}. \quad (3.65)$$

Conversely, the following Lemma holds:

Lemma 3.6. *For any m*

$$E_\varepsilon^U(m+1, L) - E_\varepsilon^U(m, L) \leq 8\pi a \frac{m}{L^3} \quad (3.66)$$

Proof. Let the operator $\tilde{H}_m$ (n replaced by m) have the ground state $\tilde{\Psi}_m$ normalised in Λ^m. Let further t_i' denote the distance from $\mathbf{x}_i$ to the nearest of its neighbours among the points $\mathbf{x}_1, ..., \mathbf{x}_{m+1}$ without $\mathbf{x}_i$, and t_i the corresponding distance excluding $\mathbf{x}_{m+1}$. It can easily be seen that

$$U(t_i') \leq U(t_i) + U(|\mathbf{x}_i - \mathbf{x}_{m+1}|) \quad (3.67)$$

and

$$U(t'_{m+1}) \leq \sum_{i=1}^{m} U(|\mathbf{x}_i - \mathbf{x}_{m+1}|). \tag{3.68}$$

Hence, for small ε we obtain the estimate

$$\tilde{H}_{m+1} \leq \tilde{H}_m - \frac{1}{2}\varepsilon\Delta_{m+1} + 2a\sum_{i=1}^{m} U(|\mathbf{x}_i - \mathbf{x}_{m+1}|). \tag{3.69}$$

If we now insert in the above inequality the trial state $\tilde{\Psi}_m/L^{3/2}$, normalised in Λ^{m+1}, noticing that $E_\varepsilon^U(m+1, L) \leq \langle\tilde{\Psi}_m/L^{3/2}, H_{m+1}\tilde{\Psi}_m/L^{3/2}\rangle$ and that $\Delta_{m+1}\tilde{\Psi}_m/L^{3/2} = 0$, since Δ_{m+1} acts on the $\mathbf{x}_{m+1}$ which is absent in $\tilde{\Psi}_m$, we obtain

$$E_\varepsilon^U(m+1, L) - E_\varepsilon^U(m, L) \leq \frac{2a}{L^3}\int \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_{m+1} \sum_{i=1}^{m} U(|\mathbf{x}_i - \mathbf{x}_{m+1}|)|\tilde{\Psi}_m|^2. \tag{3.70}$$

To finish the proof of the Lemma, we first do the $\mathbf{x}_{m+1}$ integration in spherical coordinates. This yields a factor of 4π, since the potential $U = \frac{1}{3(R^3 - R_0^3)}$ is non-zero only for $R_0 \leq r \leq R$, thereby concluding the proof of the Lemma.

□

The upper and lower bounds on $E_\varepsilon^U(\bar{n}_\alpha, L)$ require that $\bar{n}_\alpha \sim \rho_{\alpha,max}L^3$. Choosing $L \sim N^{-10}$ we find $\rho_{\alpha,max} \sim N$, whence $\bar{n}_\alpha \sim N^{7/10}$ and $Y_\alpha \sim N^{-2}$, thus fulfilling all the three conditions.

Now we are ready to do the decisive step, minimising Q_α further. To this end, consider the expression

$$4\pi a\Big(\frac{\rho_{\alpha,min}}{\rho_{\alpha,max}}(1 - CY^{1/17}) - 2n_\alpha\rho_{\alpha,max}\Big) \tag{3.71}$$

which is a lower bound to Q_α and follows directly from (3.63) and (3.64). Dropping the requirement that n_α be integer and minimising it as a function of n_α we find

$$n_\alpha = \frac{\rho_{\alpha,max}^2}{\rho_{\alpha,min}}\frac{L^3}{(1 - CY^{1/17})}. \tag{3.72}$$

By equation (3.49), together with the term for the contribution outside Λ_M and including the small error $\varepsilon C_M n_\alpha$ we obtain

$$\begin{aligned} E_0(N,a) - E^{GP}(N,a) \quad \geq \quad & 4\pi a\int|\rho^{GP}|^2 - 4\pi a\sum_{\alpha\subset\Lambda_M}\rho_{\alpha,min}^2 L^3\Big(\frac{\rho_{\alpha,max}^3}{\rho_{\alpha,min^3}}\frac{1}{(1 - CY^{1/17})}\Big) - \\ - \quad & Y^{1/17}NC_M - 4\pi aN\sup_{\mathbf{x}\notin\Lambda_M}\rho^{GP}. \end{aligned} \tag{3.73}$$

We remind that $\rho^{GP} > 0$. Since all the cells are contained in the cube Λ_M, there exist constants $C' < \infty$ and $C'' > 0$, such that

$$\rho_{\alpha,max}^3 - \rho_{\alpha,min}^3 \leq NC'L \quad \text{and} \quad \rho_{\alpha,min}^3 \geq NC''. \tag{3.74}$$

Then for $L \sim N^{-10}$, $N \geq 1$ and $Y \sim N^{-17/10}$, we have, using the above relations, for N large enough

$$\begin{aligned}&\frac{\rho^3_{\alpha,max}}{\rho^3_{\alpha,min}}\frac{1}{(1-CY^{1/17})} \leq \Big(\frac{NC'L}{\rho^3_{\alpha,min}}+1\Big)\frac{1}{(1-CN^{-1/10})}\\ \leq &\Big(1+\frac{C'}{C''}N^{-1/10}\Big)(1+O(N^{-1/10})) \leq 1+\text{const.}N^{-1/10}.\end{aligned} \tag{3.75}$$

Also,

$$4\pi a \sum_{\alpha\subset\Lambda_M} \rho^2_{\alpha,min}L^3 \leq 4\pi a \int |\rho^{GP}|^2 \leq E^{GP}(N,a). \tag{3.76}$$

Putting this in (3.73), recalling the scaling properties of the GP theory and dividing by $E^{GP}(N,a)$ yields:

$$\frac{E_0^{QM}(N,a)}{E^{GP}(N,a)} \geq 1 - \text{const.}(1+C_M)N^{-10} - \text{const.} \sup_{\mathbf{x}\notin\Lambda_M} \rho^{GP}_{1,Na}, \tag{3.77}$$

where the constants depend on the fixed parameter Na only. It remains to take the N and M limits, but we have to do it in the right order. First, take $N \to \infty$ and then $M \to \infty$ to kill the supremum term. Thus, we get

$$\liminf_{N\to\infty} \frac{E_0^{QM}(N,a)}{E^{GP}(N,a)} \geq 1. \tag{3.78}$$

□

Chapter 4

Conclusions

In this thesis we proved that the ground state energy of a weakly interacting Bose gas in the GP scaling limit is captured by the Gross-Pitaevskii non-linear theory. To this end, we discussed separately a lower and an upper bound to the ground state energy. We conclude our analysis by remarking that a the GP theory actually captures also the true asymptotics of the reduced density matrix, as shown in [13]:

Theorem 4.1. *Let Na be fixed, and let $\gamma(\boldsymbol{x}, \boldsymbol{x}')$ denote the one-particle reduced density matrix given by*

$$\gamma(\boldsymbol{x}, \boldsymbol{x}') = N \int \Psi_0^*(\boldsymbol{x}, \boldsymbol{X}) \Psi_0(\boldsymbol{x}', \boldsymbol{X}) \mathrm{d}\boldsymbol{X}, \tag{4.1}$$

with Ψ_0 denoting the ground state of (3.1). Then the following limit in the trace-class norm holds

$$tr \left| \frac{1}{N} \gamma(\boldsymbol{x}, \boldsymbol{x}') - |\phi^{GP}\rangle\langle\phi^{GP}| \right| \xrightarrow{N\to\infty} 0. \tag{4.2}$$

where ϕ^{GP} is defined in Lemma 3.1.

This proves the emergence of condensation in the limit $N \to \infty$ analogously to the non-interacting case, due to the fact that the one-particle reduced density matrix converges in the above sense to the projection onto the GP ground state.

The development of rigorous results in the theory of BEC has been drastically triggered by experimental results in the past decade. The reason why the mathematical description turned out to be so useful lies in the precise error estimates provided by the proofs, which can be experimentally confirmed to extremely high accuracy. During the last ten years, rigorous proofs have been established for the cases of one, two and three-dimensional systems with error estimates extended even up to second order in N. Furthermore, the Bose gas has been investigated also in systems under fast rotation, cigar-shaped and disc-shaped systems, just to name a few. There has been a multitude of results about the charged Bose gas as well. The longer this area of mathematical physics remains active, the better our understanding of this most peculiar phase transition will be, so that hopefully one day this knowledge can be used for the development of modern technology, present in our everyday life.

Appendix A

Notations

The following is a short list of notations used throughout the thesis. They shall make sense, whenever the objects used below are well-defined.

- $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$: coordinates of a fixed particle
- $L^2 = L^2(\mathbb{R}^3, \mathrm{d}x) := \{f : \mathbb{R}^3 \to \mathbb{C}, \text{s.t.} \int_{\mathbb{R}^3} |f(x)|^2 \mathrm{d}x\mathrm{d}x < \infty\}$: the second Lebesgue space on $\mathbb{R}^3$ over the complex numbers $\mathbb{C}$ with respect to the Lebesgue measure $\mathrm{d}x$.
- $H^1 = H^1(\mathbb{R}^3, \mathrm{d}x) := \{f : \mathbb{R}^3 \to \mathbb{C}, \text{s.t.} \int_{\mathbb{R}^3} |f(x)|^2 + |f'(x)|^2 \mathrm{d}x < \infty\}$: the first Sobolev space on $\mathbb{R}^3$ over the complex numbers $\mathbb{C}$.
- $[A, B] = AB - BA$: the commutator of two operators A,B.
- $\lim_{\mathrm{TD}} := \lim_{N,L\to\infty, N/L^3=\text{const.}}$: the thermodynamic limit

Bibliography

[1] N. N. Bogoliubov, *On the theory of superfluidity*, J. Phys. (USSR) **11** (1947), 2332.

[2] A.Yu. Cherny and A.A. Shanenko, *The kinetic and interaction energies of a trapped Bose gas: beyond the mean field*, Phys. Rev. Lett. A **293** (2002), 287292.

[3] F.J. Dyson, *Ground-state energy of a hard-sphere gas*, Phys. Rev. **106** (1957), 20–26.

[4] A. Einstein, *Quantentheorie des einatomigen idealen gases*, Sitzber. Kgl. Preuss. Akad. Wiss. (1924), 261267.

[5] R. P. Feynman, *Application of quantum mechanics to liquid helium*, in Progress in Low Temperature Physics, vol. 1, Amsterdam: North-Holland (1955), 1753.

[6] R.P. Feynman, *Statistical mechanics: A set of lectures*, Perseus Books, Reading, Massachusetts, 1972.

[7] K. Huang, *Statistical mechanics*, John Wiley&Sons, New York, 1963.

[8] S. Kehrein, *Quantenmechanik: Vorlesungsskriptum, wintersemester 07/08*, script (2008).

[9] W. Ketterle, *Nobel lecture: when atoms behave as waves: Bose-Einstein condensation and the atom laser*, Rev. Mod. Phys. **74** (2002), 11311151.

[10] L. D. Landau and E. M. Lifshitz, *Statisticheskaya fizika*, Fizmatgiz, Moscow, 1951.

[11] E.H. Lieb and M. Loss, *Analysis, 2nd ed.*, Amer. Math. Society, Providence R.I., 2001.

[12] E.H. Lieb and R. Seiringer, *Proof of Bose-Einstein condensation for dilute trapped gases*, Phys. Rev. Lett. **88** (2002), 170409–14.

[13] E.H. Lieb, R. Seiringer, J.P. Solovej, and J. Yngvason, *The mathematics of the Bose gas and its condensation*, Birkhäuser Verlag, Basel, 2005.

[14] 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** (2000), 043602.

[15] ———, *Superfluidity in dilute trapped Bose gases*, Phys. Rev. B **66** (2002), 134529.

[16] E.H. Lieb and J. Yngvason, *Ground state energy of the low density Bose gas*, Phys. Rev. Lett. **80** (1998), 25042507.

[17] ———, *Ground state energy of the low density Bose gas*, Phys. Rev. Lett. **80** (1998), 25042507.

[18] ———, *The ground state energy of a dilute twodimensional Bose gas*, J. Stat. Phys. **103** (2001), 509.

[19] F. London, *On the Bose-Einstein condensation*, Phys. Rev. **54** (1938), 947954.

[20] A. Michelangeli, *Bose-Einstein condensation: analysis of problems and rigorous results*, Ph.D. thesis, SISSA (2007).

[21] A. Michelangeli and B. Schlein, *Dynamical collapse of boson stars*, (2010).

[22] L. Onsager, *Statistical hydrodynamics*, Nuovo Cimento (9) **6** (1949), 279287.

[23] O. Penrose, *On the quantum mechanics of helium ii*, Philos. Mag. (1951).

[24] O. Penrose and L. Onsager, *Bose-Einstein condensation and liquid helium*, Phys. Rev. **104** (1956), 576584.

[25] L. Pitaevskii and S. Stringari, *Bose-Einstein condensation*, Clarendon Press, Oxford, 2003.

[26] ———, *Bose-Einstein condensation*, Clarendon Press, Oxford, 2003.

[27] M. Reed and B. Simon, *Methods of modern mathematical physics, vol. 1*, New York Academic Press, 1972.

[28] ———, *Methods of modern mathematical physics, vol. 2*, New York Academic Press, 1975.

[29] R. Seiringer, Diplom thesis, University of Vienna (1999).