Master Thesis

# Free Energy of the Dilute Bose Gas

*Author:*
David Stocker

*Supervised by:*
Prof. Dr. Benjamin Schlein
Dr. Andreas Deuchert

Universität Zürich[UZH]

Department of Mathematics
University of Zurich

January 27, 2022

## Abstract

We prove an upper bound to the grand canonical free energy $F(N, L, T)$ of the dilute Bose gas in the Gross-Pitaevskii limit given by $F(N, L, T) \leq F_0^{\text{th}}(N_{\text{th}}, L, T) + 4\pi a L^3(2\varrho^2 - \varrho_0^2) + T/2 \ln(T^{-1}4aL^{-3}) + C_\varepsilon L^{-2} N^{1/2+\varepsilon}$ for arbitrary but fixed $\varepsilon > 0$. Here $N$ denotes the expected number of particles, $L$ the side length of the box, and $a$ the scattering length of the potential. Moreover, $F_0^{\text{th}}(N_{\text{th}}, L, T)$ and $\varrho_0$ denote the free energy of the non-condensed particles and the expected condensate density of the ideal Bose gas, respectively. The bound is valid for temperatures $T$ below the critical temperature of the Bose-Einstein condensation phase transition in the ideal Bose gas. The main new contribution is the third order term originating from the entropy and the interaction energy of the condensate.

# Contents


**1 Introduction** **4**

**2 Background in Many-Body Quantum Mechanics** **8**
2.1 Second Quantization . . . . . 8
2.2 Coherent States . . . . . 16
2.3 Quantum Statistical Mechanics . . . . . 19
2.4 The Ideal Bose Gas . . . . . 23
2.5 The Scattering Equation . . . . . 26

**3 Main Result** **31**

**4 Proof of the Main Theorem** **34**
4.1 Proof Strategy . . . . . 34
4.2 Construction of the Trial State . . . . . 34
4.3 Preparatory Lemmas . . . . . 38
4.4 Particle Expectation of the Trial State . . . . . 46
4.5 Estimation of the Energy . . . . . 49
4.5.1 Interaction Energy . . . . . 50
4.5.2 Application of the Scattering Equation . . . . . 52
4.5.3 Bound for the Interaction Energy Remainder . . . . . 53
4.5.4 Bound for the Kinetic Energy Remainder . . . . . 56
4.6 Estimation of the Entropy . . . . . 58
4.7 Thermal Free Energy of the Ideal Bose Gas . . . . . 60
4.8 Combining the derived Bounds . . . . . 61

**References** **63**

# 1 Introduction

At the beginning of the twentieth century the Indian physicist S.N. Bose realized that the statistics governing photons is determined by restricting the many-photon wave function to symmetric tensor products of single photon states. Honouring Bose's insights, all particles behaving symmetrically by permutation in the many-body wave function are called bosons. Their antisymmetric counterparts are called fermions. All known particles can be divided into these two families and many physical effects can be accounted for by these exchange symmetries. One famous effect is Bose-Einstein condensation. In contrast to fermions, the permuation symmetry of bosons allows more than one particle to occupy the same state. The effect occurs usually at very low temperatures when a finite fraction of particles begin to occupy the lowest energy eigenstate. This leads to peculiar macroscopic quantum effects.
After the first experimental realization of Bose-Einstein condensate in a low density alkali gas in [1] the interest in the theoretical study of bosonic quantum gases increased a lot. Since then numerous rigorous results have been derived. However, there still remain many open problems and unresolved issues.

The goal of this thesis is to investigate energetic aspects of the dilute Bose at positive temperatures. Concretely, we will prove an upper bound to the free energy of an interacting dilute Bose gas. To motivate and rigorously formulate our goal, we outline in this introduction some of the theoretical foundations in the study of bosonic systems.

As in any quantum mechanical problem a good starting point is to consider the general Hamiltonian of the system:

$$H = \sum_{i=1}^{N} -\Delta_i + V(x_1, ..., x_N). \tag{1.0.1}$$

For convenience we normalized $2m = 1$, $\hbar = 1$.The operator $\sum_{i=1}^{N} -\Delta_i$ describes the kinetic energy of the $N$ particles in the gas. By $V(x_1, ..., x_N)$ a general interaction potential is denoted. The trivial case, where $V = 0$, describes the ideal Bose gas. The Hamiltonian acts on functions $\Psi \in \otimes_{sym}^{N} \mathcal{H}$ where $\otimes_{sym}^{N} \mathcal{H}$ denotes the $N$-fold symmetric tensor product of the one-particle Hilbert space $\mathcal{H}$. Furthermore, we assume that the Bose gas is containend in a box $\Lambda_L$ of side length $L$ with periodic boundary conditions. In this case the one-particle Hilbert space takes the form $\mathcal{H} = L^2(\mathbb{R}^3)$.
In equilibrium and at zero temperature, bosonic systems are known to minimize the energy. Thus, the ground state of the system, defined by the bosonic state $\Psi$ that attains the energetic infimum

$$E_0 = \inf_{\substack{\Psi \in \otimes_{sym}^{N} \mathcal{H} \\ \langle \Psi, \Psi \rangle = 1}} \langle \Psi, H\Psi \rangle , \tag{1.0.2}$$

is of particular interest. Unfortunately, this equation is not exactly solvable in most cases and we are not able to derive a precise expression for the groundstate energy $E_0$. Moreover, it is often even harder to determine properties of the ground state, for example, if the system shows Bose-Einstein condensation. Therefore, for the mathematical study of the system, we need to make assumptions on the potential and take limits to obtain meaningful, rigorous results.
Motivated by this, we consider here dilute Bose gases. The system is described by the Hamiltonian

$$H = \sum_{i=1}^{N} -\Delta_i + \sum_{1\leq i<j\leq N} V(x_i - x_j). \tag{1.0.3}$$

For simplicity we assume $V$ to be spherically symmetric, compactly supported and $V \geq 0$. The last assumption ensures that there are no bound states in the gas.
It is instructive to have a closer look at the scattering process of two particles. The two-particle interaction is described by the zero energy Schrödinger equation

$$\Big[ -2\Delta + V\Big]\phi(x) = 0. \tag{1.0.4}$$

The factor 2 is accounting for the reduced mass in the two-particle scattering process. It can be deducted[1] that equation (1.0.4) has a solution of the form

$$\phi_0 = 1 - \frac{a}{|x|} \tag{1.0.5}$$

for some $a \geq 0$ and for $|x| \geq R_0$ where $R_0$ is the radius of support of $V$. The constant $a$ is called the scattering length of the potential $V$. It is a combined measure for the range and strength of the potential. For $R > R_0$, we can compute the energy of the solution:

$$\int_{|x|\leq R} \Big(2|\nabla\phi_0(r)|^2 + V|\phi_0|^2\Big)dx = \int_{|x|\leq R} 2\nabla\Big(\phi_0\nabla\phi_0\Big)dx = 8\pi\left(1 - \frac{a}{R}\right) \to 8\pi a \quad \text{for } R \to \infty, \tag{1.0.6}$$

where we applied the scattering equation (1.0.4) and the Stokes theorem. Thus, the energy of two particles in the large box $\Lambda_L$ can be approximated by $8\pi a/L^3$ if $a \ll L$. Here the additional factor of $L^{-3}$ originates from an approximate normalization of the wave-function. Considering there are $N(N-1)/2$ pairs, it is reasonable to expect

$$E_0(N, L) \approx 4\pi a N(N-1)/L^3 \tag{1.0.7}$$

and therefore we expect for the energy per particle:

$$e_0(N, L) \approx 4\pi a\varrho, \tag{1.0.8}$$

where $\varrho$ is the average density. Physically, the term dilute means that the average interparticle distance $\varrho^{-1/3}$ is much larger than the scattering length $a$. This can be achieved in several ways. The most intuitive way is taking first the thermodynamic limit $N, L \to \infty$ while keeping $\varrho$ fixed and afterwards taking the dilute limit $\varrho a^3 \to 0$. In [19] (upper bound) and [20] (lower bound) it was proven that in this dilute limit we indeed have

$$\lim_{\varrho a^3\to 0} \frac{e_0(\varrho)}{4\pi\varrho a} = 1. \tag{1.0.9}$$

[1] We will prove the existence and properties of the solution in section 2.5

The works of N. N. Bogoliubov [5], [6] and others [15], [17] suggest several higher order terms:

$$\frac{e_0(\varrho)}{4\pi\varrho a} = 1 + \frac{128}{15\sqrt{\pi}}\left(\varrho a^3\right)^{1/2} + 8\left(\frac{4\pi}{3} - \sqrt{3}\right)\left(\varrho a^3\right)\ln\left(\varrho a^3\right) + O\left(\varrho a^3\right). \tag{1.0.10}$$

Up to the second order term $\frac{128}{15\sqrt{\pi}}(\varrho a^3)^{1/2}$ the equation (1.0.10) is known as the Lee-Huang-Yang formula. It has been proven by the combined works of [29], [2] (upper bound) and [12], [13] (lower bound).
The remarkable conclusion from the Lee-Huang-Yang formula is that in the dilute limit the ground state energy per particle only depends on the parameter $\varrho a^3$ up to at least the second order. Thus, the exact shape of the interaction potential seems to become irrelevant in this limit.
Another limit of interest is the Gross-Pitaevskii (GP) limit. In this regime, the interaction is of the same order of magnitude as the spectral gap of the Laplacian. Specifically, we write our Hamiltonian in the following way:

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1\le i<j\le N}^{N} (N/L)^2 V(N(x_i - x_j)/L). \tag{1.0.11}$$

A quick computation shows that the scattering length rescales to $a_N = a_V L/N$. We investigate $H_N$ in the limit $N \to \infty$ with $L$ fixed.
The GP limit can be interpreted as a combined thermodynamic and dilute limit. Therefore it does not surprise that the same asymptotics as in (1.0.10) up to second order were rigorously justified in [3] for the GP limit. It should also be noted that in modern experiments Bose gases are studied in trapping potentials. According to [9], the GP limit describes this setting well. Furthermore, rigorous results are often easier to prove in this limit. This is due to the fact that this regime is an even more dilute limit than taking first the thermodynamic limit and then considering $\varrho a^3 \to 0$.
For a better understanding of modern experiments it is vital to include temperature dependencies into the analysis. Accordingly, we study the free energy of the system given by the Gibbs variational principle

$$F(N, L, \beta) = \inf_{\Gamma\in\mathscr{S}_N} \left\{ \mathrm{Tr}\left[H\Gamma\right] - \frac{1}{\beta}S(\Gamma)\right\} \tag{1.0.12}$$

where the trace is taken over $\otimes_{sym}^{N}\mathcal{H}$ and the infimum is taken over all states in the set $\mathscr{S}_N = \{\Gamma \in \mathcal{B}(\otimes_{sym}^{N}\mathcal{H}) \mid 0 \le \Gamma, \mathrm{Tr}[\Gamma] = 1, \mathrm{Tr}[\Gamma H] < \infty\}$. Moreover, we define $\beta := T^{-1}$ where $T$ is the temperature and the Boltzmann constant $k_B$ is set to 1. The free energy can be interpreted as the work the system at temperature $T$ can do. For an appropriate Hamiltonian and fixed $N$ and $\beta$ it can be shown that the free energy equals

$$F(N, L, \beta) = -\frac{1}{\beta}\ln\left(\mathrm{Tr}\left[\exp(-\beta H)\right]\right). \tag{1.0.13}$$

However, analogue to the zero temperature case, this expression can only be computed explicitly in a few trivial cases. Therefore we are again forced to merely derive approximations.
As we will show in section 2.4, the temperature at which the ideal Bose gas begins to show Bose-Einstein condensation is in the order of magnitude of $\varrho^{2/3}$. Thus, it is reasonable to keep $\beta\varrho^{2/3}$ fixed in the dilute limit.

Asymptotics of the free energy in the thermodynamic limit have been derived in [22] (lower bound) and [30] (upper bound):

$$f(\varrho,\beta) = f_0(\varrho,\beta) + 4\pi a\Big(2\varrho^2 - \varrho_0^2\Big)\Big(1 + o(1)\Big). \tag{1.0.14}$$

Here $f(\varrho,\beta)$ denotes the free energy per unit volume of the interacting system and $f_0(\beta,\varrho)$ the corresponding one of the non-interacting system. Moreover, $\varrho_0$ is the condensate density. In [9] the same two-term expansion has been obtained in the GP limit. In the same paper Bose-Einstein condensation in the GP limit has been proved. The corresponding result in the thermodynamic limit still remains an unsolved problem. Furthermore, no third order contribution has been rigorously derived for the free energy in the GP or the thermodynamic limit.

As already mentioned, the main goal of this thesis is to proof an upper bound for the grand canonical free energy in the GP limit. As it turns out we are able to capture the correct first and second order terms. Furthermore, we are able to derive a third order contribution arising from the entropy. It should be noted that this entropy contribution would vanish in the thermodynamic limit. Our proof yields a better error as obtained in [9] and is inspired by [2], [8], [29] and [30].
In chapter 2 the relevant concepts and formalisms, that are needed to prove the main result, are introduced and discussed. The setting, the main result and its discussion is found in chapter 3. The proof is formulated in chapter 4.

## Acknowledgements

I would like to thank Prof. Benjamin Schlein und Dr. Andreas Deuchert for giving me the opportunity to write my thesis about this interesting topic. Especially, I want to thank Dr. Deuchert for guiding me throughout the thesis and giving me a little insight into his research. I'm very grateful that he always took plenty of time for discussions and answered my questions.
My gratitude also goes to my family and friends who supported me in many ways throughout my thesis and generally throughout my studies. I could always count on their support and their encouragement in tough times.
Last but not least, I want to thank Tabea Nydegger and Yolanda Bernet for their valuable corrections and remarks on the text.

# 2 Background in Many-Body Quantum Mechanics

## 2.1 Second Quantization

Second quantization is an important tool for studying many-body problems where the number of particles is not fixed. We will only describe here the formalism for bosonic systems. The material for this section is taken from chapter 1, 6, 7 and 8 of the lecture notes by Solovej [24]. The proof for Lemma 2.1.2 is taken from [27] and adjusted to the bosonic case.
Starting with the one-particle separable Hilbert space $\mathcal{H}$ we first want to define the bosonic Fock space $\mathscr{F}^B(\mathcal{H})$. $N$ particle systems with arbitrary symmetry can naturally be described by the $N$-fold tensor product $\mathcal{H}_N := \bigotimes^N \mathcal{H}$ of the Hilbert space $\mathcal{H}$. We will call an element $u_1 \otimes ... \otimes u_N \in \mathcal{H}_N$ a pure tensor product. As we want to restrict our system to symmetric $N$-particle wave functions we define the following operator.

**Definition 2.1.1.** For $N \in \mathbb{N}_+$ we define $P_+^N : \mathcal{H}_N \to \mathcal{H}_N$ by

$$P_+^N := \frac{1}{N!} \sum_{\sigma \in S_N} U_\sigma, \tag{2.1.1}$$

where $S_N$ is the group of permutations acting on $N$ elements and $U_\sigma : \mathcal{H}_N \to \mathcal{H}_N$ acts as

$$U_\sigma u_1 \otimes ... \otimes u_N = u_{\sigma^{-1}(1)} \otimes ... \otimes u_{\sigma^{-1}(N)} \tag{2.1.2}$$

on a pure tensor product $u_1 \otimes ... \otimes u_N$. Moreover, $P_+ : \bigoplus_{N\geq 0} \mathcal{H}_N \to \bigoplus_{N\geq 0} \mathcal{H}_N$ is the unique linear operator s.t. for any $N \in \mathbb{N}_+$ the restriction of $P_+$ to $\mathcal{H}_N$ is equal to $P_+^N$.

It is easy to see that the operators $U_\sigma$ for $\sigma \in S_N$ are unitary and that $P_+^N$ is an orthogonal projection for any $N \in \mathbb{N}$. Taking the direct sum over all symmetrized $N$-particle Hilbert spaces $P_+^N(\mathcal{H}_N)$ we define the bosonic Fock space $\mathscr{F}^B(\mathcal{H})$.

**Definition 2.1.2.** The bosonic Fock space $\mathscr{F}^B(\mathcal{H})$ is defined as

$$\mathscr{F}^B(\mathcal{H}) := \bigoplus_{N\geq 0} P_+^N \left( \bigotimes^N \mathcal{H} \right), \tag{2.1.3}$$

where the space $\bigotimes^0 \mathcal{H}$ is interpreted as $\mathbb{C}$ and the element $1 \in \mathbb{C}$ is refered to as the vacuum vector $\Omega$.

**Remark 2.1.1.** We assumed that our Hilbert space $\mathcal{H}$ is separable, which in fact implies that the corresponding Fock space $\mathscr{F}^B(\mathcal{H})$ is also a separable Hilbert space. Thus, we find a countable basis $\{\psi_\alpha\}_{\alpha=1}^\infty \subset \mathscr{F}^B(\mathcal{H})$ s.t. for given $x$ we have

$$\left\| \sum_{\alpha=1}^{n} \lambda_\alpha \psi_\alpha - x \right\| \xrightarrow{n\to\infty} 0, \tag{2.1.4}$$

for suitable coefficients $\{\lambda_\alpha\}_{\alpha=1}^\infty$.

The bosonic Fock space has the property that we can identify the Fock space of the direct sum of two one-particle spaces $\mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)$ with the tensor product of the two corresponding Fock spaces $\mathscr{F}^B(\mathcal{H}_1) \otimes \mathscr{F}^B(\mathcal{H}_2)$. The following Lemma formulates this fact.

**Lemma 2.1.1.** *Let $\mathcal{H}_1$, $\mathcal{H}_2$ be two Hilbert spaces. Then there exists a unique unitary map*

$$U : \mathscr{F}^B(\mathcal{H}_1) \otimes \mathscr{F}^B(\mathcal{H}_2) \to \mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)$$

*such that*

$$U(\Phi_1 \otimes \Phi_2) = \sqrt{\frac{(N_1+N_2)!}{N_1!N_2!}} P_+^{N_1+N_2}(\Phi_1 \otimes \Phi_2)$$

*for $\Phi_1$ belonging to the $N_1$-particle sector of $\mathscr{F}^B(\mathcal{H}_1)$ and $\Phi_2$ belonging to the $N_2$-particle sector of $\mathscr{F}^B(\mathcal{H}_2)$.*

*Proof.* It is clear that $U(\Phi_1 \otimes \Phi_2)$ is a unique element of $\mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)$. Thus the map is well-defined. Moreover, let $\Psi_1, \Phi_1$ be in the $N_1$-particle sector of $\mathscr{F}^B(\mathcal{H}_1)$ and let $\Psi_2, \Phi_2$ be in the $N_2$-particle sector of $\mathscr{F}^B(\mathcal{H}_2)$ (if $\Psi_1, \Phi_1$ resp. $\Psi_2, \Phi_2$ are not in the same sector then the inner product is zero). Then we have

$$\begin{aligned}
\langle U(\Phi_1 \otimes \Phi_2), U(\Psi_1 \otimes \Psi_2) \rangle_{\mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)} &= \frac{(N_1+N_2)!}{N_1!N_2!} \langle P_+^{N_1+N_2}(\Phi_1 \otimes \Phi_2), P_+^{N_1+N_2}(\Psi_1 \otimes \Psi_2) \rangle_{\mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)} \\
&= \frac{(N_1+N_2)!}{N_1!N_2!} \langle P_+^{N_1+N_2}(\Phi_1 \otimes \Phi_2), \Psi_1 \otimes \Psi_2 \rangle_{\mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)} \\
&= \langle P_+^{N_1}(\Phi_1) \otimes P_+^{N_2}(\Phi_2), \Psi_1 \otimes \Psi_2 \rangle_{\mathscr{F}^B(\mathcal{H}_1) \otimes \mathscr{F}^B(\mathcal{H}_2)}.
\end{aligned}$$

Thus the map $U$ is unitary. The uniqueness follows because we can choose a complete orthonormal set of vectors in $\mathscr{F}^B(\mathcal{H}_1 \oplus \mathcal{H}_2)$ that are of the form $P_+^{N_1+N_2}(\Phi_1 \otimes \Phi_2)$ such that $\Phi_1$ belongs to the $N_1$-particle sector of $\mathscr{F}^B(\mathcal{H}_1)$ and $\Phi_2$ belongs to the $N_2$-particle sector of $\mathscr{F}^B(\mathcal{H}_2)$. □

The symmetrization procedure in many-body systems is often a tedious task. To describe the system, it is often easier to just give the information of how many particles are in each eigenstate of the system. As we are interested in systems with a variable particle number it is useful to define operators that create or annihilate particles from the system while preserving the bosonic symmetry.

**Definition 2.1.3.** Let $f \in \mathcal{H}$, we define the creation operator $a^*(f) : \mathscr{F}(\mathcal{H}) \to \mathscr{F}(\mathcal{H})$ and the annihilation operator $a(f) : \mathscr{F}(\mathcal{H}) \to \mathscr{F}(\mathcal{H})$ by the action on a pure tensor product in $\mathcal{H}_N$ given by

$$a^*(f)(f_1 \otimes ... \otimes f_N) = (N+1)^{1/2} f \otimes f_1 \otimes ... \otimes f_N, \tag{2.1.5}$$

$$a(f)(f_1 \otimes ... \otimes f_N) = N^{1/2} \langle f, f_1 \rangle f_2 \otimes ... \otimes f_N, \tag{2.1.6}$$

where $\langle , \rangle$ is the inner product of the space $\mathcal{H}$. The bosonic creation and annihilation operators on the bosonic Fock space $\mathscr{F}^B(\mathcal{H})$ are then defined as

$$a_+^*(f) := P_+ a^*(f), \qquad a_+(f) := a(f). \tag{2.1.7}$$

Note that it was only necessary to apply the symmetrizing operator $P_+$ on the creation operator. This comes from the fact that annihilating a particle from a symmetrized state keeps the final state symmetrized.
In the following Lemma we collect some basic properties of $a_+^*(f)$ and $a_+(f)$.

**Lemma 2.1.2.** *Let $f, g \in \mathcal{H}$ and define the commutator of two operators $A, B$ by $[A, B] := AB - BA$. Then we have:*

1. *The map $f \to a_+^*(f)$ is linear whereas the map $f \to a_+(f)$ is anti-linear.*
2. *$a_+^*(f), a_+(f)$ are adjoint to each other, i.e. $\langle \psi, a_+(f)\phi \rangle = \langle a_+^*(f)\psi, \phi \rangle$ for all $\psi, \phi \in \mathscr{F}^B(\mathcal{H})$.*
3. *We have the canonical commutation relations*

$$[a_+(f), a_+(g)] = [a_+^*(f), a_+^*(g)] = 0, \quad [a_+(f), a_+^*(g)] = \langle f, g \rangle I. \tag{2.1.8}$$

*Proof.* 1. The first statement follows directly from the definition of the creation and annihilation operators.
2. Fix $N \in \mathbb{N}_+$ and let $g_1 \otimes ... \otimes g_{N-1} \in \mathcal{H}_{N-1}$, $f_1 \otimes ... \otimes f_N \in \mathcal{H}_N$ be two pure tensor products. We also take $g_N \in \mathcal{H}$. Using that $(P_+^N)^* = P_+^N$, we get

$$\begin{aligned}
\langle P_+^N a^*(g_N) g_1 \otimes ... \otimes g_{N-1}, f_1 \otimes ... \otimes f_N \rangle &= \langle a^*(g_N) g_1 \otimes ... \otimes g_{N-1}, P_+^N f_1 \otimes ... \otimes f_N \rangle \\
&= \frac{N^{1/2}}{N!} \sum_{\sigma \in S_N} \langle g_N \otimes g_1 \otimes ... \otimes g_{N-1}, f_{\sigma^{-1}(1)} \otimes ... \otimes f_{\sigma^{-1}(N)} \rangle \\
&= \frac{N^{1/2}}{N!} \sum_{\sigma \in S_N} \langle g_N, f_{\sigma^{-1}(1)} \rangle \langle g_1 \otimes ... \otimes g_{N-1}, f_{\sigma^{-1}(2)} \otimes ... \otimes f_{\sigma^{-1}(N)} \rangle \\
&= \langle g_1 \otimes ... \otimes g_{N-1}, a(g_N) P_+^N f_1 \otimes ... \otimes f_N \rangle .
\end{aligned}$$

By bilinearity of the inner product we get for every $g, h \in \mathcal{F}(H)$ and $f \in \mathcal{H}$

$$\langle P_+ a^*(f) g, h \rangle = \langle g, a(f) P_+ h \rangle .$$

As we have $P_+ a^*(f) = P_+ a^*(f) P_+$ we get for $g, h \in \mathcal{F}^B(H)$ and $f \in \mathcal{H}$

$$\langle a_+^*(f) g, h \rangle = \langle g, a_+(f) h \rangle .$$

3. We assume $N \geq 2$ for the annihilation commutator. The case $N \in \{0, 1\}$ is trivial as we have $a(f)a(g)\Omega = 0$ and $a(f)a(g)h = 0$ for $f, g, h \in \mathcal{H}$. We write for a pure tensor $h_1 \otimes ... \otimes h_N \in \mathcal{H}_N$

$$\begin{aligned} a_+(f)a_+(g)P_+^N h_1 \otimes ... \otimes h_N &= \frac{(N-1)^{1/2}N^{1/2}}{N!} \sum_{\sigma \in S_N} \langle g, h_{\sigma^{-1}(1)} \rangle \langle f, h_{\sigma^{-1}(2)} \rangle h_{\sigma^{-1}(3)} \otimes ... \otimes h_{\sigma^{-1}(N)} \\ &= \frac{(N-1)^{1/2}N^{1/2}}{N!} \sum_{\sigma \in S_N} \langle f, h_{\sigma^{-1}(1)} \rangle \langle g, h_{\sigma^{-1}(2)} \rangle h_{\sigma^{-1}(3)} \otimes ... \otimes h_{\sigma^{-1}(N)} \\ &= a_+(g)a_+(f)P_+^N h_1 \otimes ... \otimes h_N. \end{aligned}$$

Using bilinearity $[a_+(f), a_+(g)] = 0$ follows.
The commutator of the bosonic creation operators follows similarly

$$\begin{aligned} a_+^*(f)a_+^*(g)P_+^N h_1 \otimes ... \otimes h_N &= (N+2)^{1/2}(N+1)^{1/2}P_+^{N+2} f \otimes \left(P_+^{N+1} g \otimes (P_+^N h_1 \otimes ... \otimes h_N)\right) \\ &= (N+2)^{1/2}(N+1)^{1/2}P_+^{N+2} f \otimes g \otimes h_1 \otimes ... \otimes h_N \\ &= (N+2)^{1/2}(N+1)^{1/2}P_+^{N+2} g \otimes \left(P_+^{N+1} f \otimes (P_+^N h_1 \otimes ... \otimes h_N)\right) \\ &= a_+^*(g)a_+^*(f)P_+^N h_1 \otimes ... \otimes h_N. \end{aligned}$$

To prove the statement for the commutator of the creation with the annihilation operator we compute

$$\begin{aligned} a_+(f)a_+^*(g_N)P_+^{N-1} g_1 \otimes ... \otimes g_{N-1} &= \frac{1}{(N-1)!} \sum_{\sigma \in S_N} \langle f, g_{\sigma^{-1}(N)} \rangle g_{\sigma^{-1}(1)} \otimes ... \otimes g_{\sigma^{-1}(N-1)} \\ &= \frac{1}{(N-1)!} \sum_{\substack{\sigma \in S_N \\ \sigma^{-1}(N) \neq N}} \langle f, g_{\sigma^{-1}(N)} \rangle g_{\sigma^{-1}(1)} \otimes ... \otimes g_{\sigma^{-1}(N-1)} \\ &\quad + \frac{1}{(N-1)!} \sum_{\substack{\sigma \in S_N \\ \sigma^{-1}(N) = N}} \langle f, g_N \rangle g_{\sigma^{-1}(1)} \otimes ... \otimes g_{\sigma^{-1}(N-1)} \\ &= a_+^*(g_N)a_+(f)P_+^{N-1} g_1 \otimes ... \otimes g_{N-1} + \langle f, g_N \rangle P_+^{N-1} g_1 \otimes ... \otimes g_{N-1}. \end{aligned}$$

With this the statement follows by bilinearity. □

The great advantage of the second quantization formalism is that we can express symmetric operators acting on the Fock space $\mathscr{F}^B(\mathcal{H})$ in terms of creation and annihilation operators. In the following we will see how the second quantization of one-particle and two-particle operators are written.
We first need to define how one-particle and two-particle operators generalize onto $\mathscr{F}^B(\mathcal{H})$. This generalization is called the second quantization of a one-particle respectively two-particle operator. As we only work with bosonic particles we denote from now on by $\mathscr{F}(\mathcal{H})$ the bosonic Fock space.

**Definition 2.1.4.** The second quantization of a one-particle operator $H$ is defined as

$$d\Gamma(H) := \bigoplus_{N=1}^{\infty} H_N. \tag{2.1.9}$$

Here we denote $H_N = \sum_{j=1}^N I^{\otimes j-1} \otimes H \otimes I^{\otimes N-j}$.

**Example 2.1.1.** On a $n$-fold symmetric tensor product the number operator $\mathcal{N}$ is defined as follows

$$\mathcal{N}P_+^n(f_1 \otimes ... \otimes f_n) = nP_+^n(f_1 \otimes ... \otimes f_n).$$

It is easy to see that $\mathcal{N} = d\Gamma(I)$ on the Fock space $\mathscr{F}(\mathcal{H})$.

In the following we denote by $X_{i,j} : \mathcal{H}_N \to \mathcal{H}_N$ the unitary corresponding to a simple interchange of the $i$-th with the first and the $j$-th with the second tensor factor.

**Definition 2.1.5.** The second quantization of a two-particle operator $V$ is defined as

$$d\Gamma(V) := \bigoplus_{N=2}^{\infty} V_N. \tag{2.1.10}$$

Here we denote $V_N = \sum_{1\le i<j\le N} V_{i,j} = \sum_{1\le i<j\le N} X_{i,j}(V \otimes I^{\otimes N-2})X_{i,j}$.

**Lemma 2.1.3.** *Let $H$ be a symmetric operator on $\mathcal{H}$ and let $\{u_\alpha\}_{\alpha=1}^{\infty}$ be an orthonormal basis for $\mathcal{H}$ with elements from the domain $D(H)$. We may then write*

$$d\Gamma(H) = \sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty} \langle u_\alpha, Hu_\beta\rangle\, a_+^*(u_\alpha)a_+(u_\beta) \tag{2.1.11}$$

*as quadratic forms on the domain $\bigcup_{M=0}^{\infty}\bigoplus_{N=1}^{M} P_+^N D\Big(\sum_{j=1}^N H_j\Big)$ (for M=0 the domain is $\mathbb{C}$).*

*Proof.* Using that $\{u_\alpha\}_{\alpha=1}^{\infty}$ is an orthonormal basis, we can write for $f, g \in D(H)$

$$\begin{aligned}\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty} \langle g, u_\alpha\rangle \langle u_\alpha, Hu_\beta\rangle \langle u_\beta, f\rangle &= \sum_{\beta=1}^{\infty} \langle g, Hu_\beta\rangle \langle u_\beta, f\rangle = \sum_{\beta=1}^{\infty} \langle Hg, u_\beta\rangle \langle u_\beta, f\rangle \\ &= \langle Hg, f\rangle = \langle g, Hf\rangle .\end{aligned}$$

This shows that the claim (2.1.11) holds in the sense of quadratic forms on $D(H)$.
Now consider the action of $a^*(u_\alpha)a(u_\beta)$ on a pure tensor product

$$a^*(u_\alpha)a(u_\beta)f_1 \otimes ... \otimes f_N = N\langle u_\beta, f_1\rangle\, u_\alpha \otimes f_2 \otimes ... \otimes f_N$$

where $f_1, ..., f_N \in D(H)$. Denote $H_j = 1^{\otimes j-1} \otimes H \otimes 1^{\otimes N-j}$. Then we have

$$\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty} \langle u_\alpha, Hu_\beta\rangle\, a^*(u_\alpha)a(u_\beta) = NH_1$$

as quadratic forms on finite linear combinations of $N$-fold pure tensor products of vectors on $D(H)$. Since $P_+$ projects onto symmetrized vectors we have $P_+NH_1P_+ = P_+\sum_{j=1}^N H_jP_+ = \sum_{j=1}^N H_jP_+$ on $\bigotimes^N \mathcal{H}$. Which gives

$$\begin{aligned}\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty} \langle u_\alpha, Hu_\beta\rangle\, a^*(u_\alpha)a(u_\beta)P_+ &= \sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty} \langle u_\alpha, Hu_\beta\rangle\, P_+a^*(u_\alpha)a(u_\beta)P_+ \\ &= d\Gamma(H)P_+\end{aligned}$$

□

**Lemma 2.1.4.** *Let $\{u_\alpha\}_{\alpha=1}^\infty$ be an orthonormal basis of $\mathcal{H}$. Let $V$ be a two-body potential for identical particles, i.e. a symmetric operator on $\mathcal{H}\otimes\mathcal{H}$ such that $X_{2,1}VX_{2,1} = V$. Assume that $u_\alpha \otimes u_\beta \in D(V)$ for all $\alpha,\beta = 1,2,....$ Then as quadratic forms on finite linear combinations of pure symmetric tensor products of basis vectors form $\{u_\alpha\}_{\alpha=1}^\infty$ we have*

$$d\Gamma(V) = \frac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha\otimes u_\beta, Vu_\mu\otimes u_\nu\rangle\, a_+^*(u_\alpha)a_+^*(u_\beta)a_+(u_\mu)a_+(u_\nu). \tag{2.1.12}$$

*Proof.* Using that $\{u_\alpha\}_{\alpha=1}^\infty$ is an orthonormal basis we can write

$$Vu_1\otimes u_2 = \sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha\otimes u_\beta, Vu_\mu\otimes u_\nu\rangle \langle u_\mu,u_1\rangle\langle u_\nu,u_2\rangle\, u_\alpha\otimes u_\beta$$

and

$$a^*(u_\alpha)a^*(u_\beta)a(u_\nu)a(u_\mu)u_1\otimes ...\otimes u_N = N(N-1)\langle u_\mu,u_1\rangle\langle u_\nu,u_2\rangle\, u_\alpha\otimes u_\beta\otimes u_3\otimes ...\otimes u_N.$$

Since this is true for any $N$-fold tensor product of basis vectors we conclude on such tensor products

$$\frac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha\otimes u_\beta, Vu_\mu\otimes u_\nu\rangle\, a^*(u_\alpha)a^*(u_\beta)a(u_\mu)a(u_\nu) = \frac{N(N-1)}{2}V_{12}.$$

As in the previous proof we have on $N$-fold tensor products

$$\frac{N(N-1)}{2}P_+V_{12}P_+ = \sum_{1\le i<j\le N} V_{i,j}P_+$$

where we used $X_{2,1}VX_{2,1} = V$. As symmetrizing after creating an extra particle makes it unnecessary to symmetrize before creating it, we have $P_+a^*(f)P_+ = P_+a^*(f)$. Thus

$$\begin{aligned}
d\Gamma(V) &= \bigoplus_{N=2}^\infty \sum_{1\le i<j\le N} V_{ij}P_+ = \bigoplus_{N=2}^\infty \frac{N(N-1)}{2}P_+V_{12}P_+ \\
&= P_+\frac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha\otimes u_\beta, Vu_\mu\otimes u_\nu\rangle\, a^*(u_\alpha)a^*(u_\beta)a(u_\mu)a(u_\nu)P_+ \\
&= \frac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha\otimes u_\beta, Vu_\mu\otimes u_\nu\rangle\, P_+a^*(u_\alpha)P_+a^*(u_\beta)a(u_\mu)a(u_\nu)P_+ \\
&= \frac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha\otimes u_\beta, Vu_\mu\otimes u_\nu\rangle\, a_+^*(u_\alpha)a_+^*(u_\beta)a_+(u_\mu)a_+(u_\nu)P_+
\end{aligned}$$

□

Using the creation and annihilation operators we can define the $n$-particle density matrix $\gamma_\Psi^{(n)}$ of a vector $\Psi\in\mathscr{F}(\mathcal{H})$. We will see that the operator $\gamma_\Psi^{(n)}$ captures a lot of the useful information of the vector $\Psi$.

**Definition 2.1.6.** Let $\Psi \in \mathscr{F}(\mathcal{H})$ be a normalized vector and assume

$$\langle \Psi, \mathcal{N}^n \Psi \rangle < \infty \tag{2.1.13}$$

where $n \in \mathbb{N}_+$. Then the $n$-particle density matrix ($n$-pdm) of $\Psi$ is defined as the operator $\gamma_\Psi^{(n)}$ on the $n$-body space $\mathcal{H}^{\otimes n}$ given by

$$\langle f_1 \otimes ... \otimes f_n, \gamma_\Psi^{(n)} g_1 \otimes ... \otimes g_n \rangle = \langle \Psi, a_+^*(g_n)...a_+^*(g_1)a_+(f_1)...a_+(f_n)\Psi \rangle \tag{2.1.14}$$

where $f_1, ..., f_n, g_1, ..., g_n \in \mathcal{H}$.

Let us show that the definition (2.1.14) indeed defines an operator. We have the sesquimultilinear form $Q : D(Q) \times D(Q) \to \mathbb{C}$ with $D(Q) \subseteq \mathcal{H}^{\otimes n}$ given by

$$Q(f_1 \otimes ... \otimes f_n, g_1 \otimes ... \otimes g_n) = \langle \Psi, a_+^*(g_n)...a_+^*(g_1)a_+(f_1)...a_+(f_n)\Psi \rangle .$$

Define the domain

$$D\left(\gamma_\Psi^{(n)}\right) := \left\{ f \in D(Q) : \sup_{g \in D(Q)\setminus\{0\}} \frac{|Q(g,f)|}{\|g\|} < \infty \right\}.$$

Then the map $g \mapsto Q(g, f)$ defines a continuous linear functional. Thus by the Riesz representation theorem we find a unique $f' \in \mathcal{H}^{\otimes n}$ such that $Q(g, f) = \langle g, f' \rangle$. Define $\gamma_\Psi^{(n)}(f) := f'$. It is easy to see that $\gamma_\Psi^{(n)}(f)$ is multilinear. Thus we find a unique multilinear map $\gamma_\Psi^{(n)} : D\left(\gamma_\Psi^{(n)}\right) \to \mathcal{H}^{\otimes n}$ such that $Q(g, f) = \langle g, \gamma_\Psi^{(n)} f \rangle$.
It is clear that the operator $\gamma_\Psi^{(n)}$ is positive semi-definite. Moreover we have for the 1-pdm

$$\mathrm{Tr}\,[\gamma_\Psi^{(1)}] = \sum_{j=1}^{\infty} \langle \Psi, a_+^*(f_j)a_+(f_j)\Psi \rangle = \langle \Psi, \mathcal{N}\Psi \rangle$$

and similarly (using additionally once the canonical commutation relations)

$$\mathrm{Tr}\,[\gamma_\Psi^{(2)}] = \langle \Psi, \mathcal{N}(\mathcal{N}-1)\Psi \rangle .$$

Moreover, we can express the expected value of a state $\Psi$ in a two-body potential using the 2-pdm

$$\begin{aligned} \langle \Psi, d\Gamma(V)\Psi \rangle &= \frac{1}{2} \sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha \otimes u_\beta, V u_\mu \otimes u_\nu \rangle \langle \Psi, a_+^*(u_\alpha)a_+^*(u_\beta)a_+(u_\mu)a_+(u_\nu)\Psi \rangle \\ &= \frac{1}{2} \sum_{\alpha,\beta,\mu,\nu=1} \langle u_\alpha \otimes u_\beta, V u_\mu \otimes u_\nu \rangle \langle u_\mu \otimes u_\nu, \gamma_\Psi^{(2)} u_\beta \otimes u_\alpha \rangle . \end{aligned}$$

The expression of the expected value of a state with an one-body Hamiltonian works similarly. Furthermore, using the 1-pdm we can rigorously define Bose-Einstein condensation (BEC):[1]

[1] The definition is taken from [9]

**Definition 2.1.7.** A sequence of states $\Psi_N$ displays BEC if the related 1-pdm $\gamma_N^{(1)}$ has at least one eigenvalue of order $N$, i.e.

$$\liminf_{N\to\infty} \frac{\sup_{\|\phi\|=1} \langle \phi, \gamma_N^{(1)} \phi \rangle}{N} > 0. \tag{2.1.15}$$

To conclude this section, we consider the example of a bosonic gas in the box $\Lambda_L := [-L/2, L/2]^3$ with periodic boundary conditions. Furthermore, we assume a grand canonical setting, i.e. the number of particles is not fixed. If a nonnegative, compactly supported two-body interaction potential $V \in L^3(\mathbb{R}^3)$ is present, then the Hamiltonian takes the form

$$H_N = -\sum_{j=1}^{N} \Delta_{x_j} + \sum_{1\le j<i\le N} V(x_i - x_j) \tag{2.1.16}$$

when acting on the Hilbert space $\mathcal{H}_N = \bigotimes_{sym}^N L^2(\Lambda_L)$.
Fourier analysis tells us that $\{u_p\}_{p\in(2\pi/L)\mathbb{Z}^3}$ with $u_p = \frac{1}{L^{3/2}} \exp(ipx)$ is an orthonormal basis of $L^2(\Lambda_L)$. Applying Lemma 2.1.11 we can write for the one-particle operator $-\Delta$:

$$d\Gamma(-\Delta) = \sum_{p,q\in(2\pi/L)\mathbb{Z}^3} \langle u_p, -\Delta u_q \rangle \, a_+^*(u_p) a_+(u_q) = \sum_{p\in(2\pi/L)\mathbb{Z}^3} p^2 a_p^* a_p. \tag{2.1.17}$$

Here we used that $\{u_p\}_{p\in(2\pi/L)\mathbb{Z}^3}$ are eigenfunctions of $-\Delta$ and denoted $a_+^*(u_p) = a_p^*$, $a_+(u_p) = a_p$. Similarly we find

$$\mathcal{N} = \sum_{p\in(2\pi/L)\mathbb{Z}^3} a_p^* a_p. \tag{2.1.18}$$

Using Lemma 2.1.4 we can express the interaction potential as

$$d\Gamma(V) = \frac{1}{2} \sum_{p,q,v,w\in(2\pi/L)\mathbb{Z}^3} \langle u_p \otimes u_q, V u_v \otimes u_w \rangle \, a_p^* a_q^* a_v a_w$$

Using the fact that we can identify $L^2(\Lambda_L, \lambda) \otimes L^2(\Lambda_L, \lambda)$ with $L^2(\Lambda_L \times \Lambda_L, \lambda \times \lambda)$ where $\lambda$ is the Lebesgue measure, we can write for the matrix element

$$\begin{aligned}
\langle u_p \otimes u_q, V u_v \otimes u_w \rangle &= \frac{1}{L^6} \int_{\Lambda_L} \int_{\Lambda_L} \exp(i(px+qy)) V(x-y) \exp(-i(vx+wy)) dx dy \\
&= \frac{1}{L^6} \int_{\Lambda_L} \int_{\Lambda_L} \exp(-iR(v+w-p-q)) V(r) \exp(-ir/2(v-p-w+q)) dR dr \\
&= \frac{1}{L^3} \delta_{p+q,v+w} \int_{\Lambda_L} V(r) \exp(-ir(v-p)) dr.
\end{aligned}$$

In the second equality we performed the change of variables $R = (x+y)/2$ and $r = x - y$, which yields $x = R + r/2$ and $y = R - r/2$. Using this we obtain

$$\begin{aligned}
d\Gamma(V) &= \frac{1}{2L^3} \sum_{p,q,v,w\in(2\pi/L)\mathbb{Z}^3} \delta_{p+q,v+w} \hat{V}(v-p) a_p^* a_q^* a_v a_w \\
&= \frac{1}{2L^3} \sum_{u,v,p\in(2\pi/L)\mathbb{Z}^3} \hat{V}(p) a_{u+p}^* a_{v-p}^* a_u a_v.
\end{aligned} \tag{2.1.19}$$

Combining (2.1.17) and (2.1.19) we can write the second quantization of the Hamiltonian (3.0.5) as

$$d\Gamma(H) = \sum_{p\in(2\pi/L)\mathbb{Z}^3} p^2 a_p^* a_p + \frac{1}{2L^3} \sum_{u,v,p\in(2\pi/L)\mathbb{Z}^3} \hat{V}(p) a_{u+p}^* a_{v-p}^* a_u a_v. \tag{2.1.20}$$

Moreover, due to Lemma 2.1.2 the bosonic creation and annihilation operators satisfy the following canonical commutation relations

$$[a_p, a_q] = [a_p^*, a_q^*] = 0, \qquad [a_p, a_q^*] = \delta_{p,q} I. \tag{2.1.21}$$

## 2.2 Coherent States

In this section we introduce coherent states on the bosonic Fock space $\mathscr{F}(\mathcal{H})$ which will later be useful to model the condensate of the Bose gas. The material for this section is taken from chapter 10.3 in [7].
From now on, for convenience, we omit to write the index + for the bosonic creation and annihilation operators. Bosonic coherent states on the Fock space $\mathscr{F}(\mathcal{H})$ are defined by the action of the Weyl operators on the vacuum state:

**Definition 2.2.1.** For $f \in \mathcal{H}$ its corresponding Weyl operator is defined by

$$W(f) := \exp\left(a^*(f) - a(f)\right). \tag{2.2.1}$$

The coherent state $\psi(f) \in \mathscr{F}(\mathcal{H})$ is then defined as

$$\psi(f) := W(f)\Omega. \tag{2.2.2}$$

We can express the coherent state $\psi(f)$ as a linear combination of $\{f^{\otimes n}\}_{n=0}^{\infty}$ where $f^{\otimes n}$ is the pure $n$-fold tensor product $f \otimes ... \otimes f$.

**Lemma 2.2.1.** *For every $f \in \mathcal{H}$ we have*

$$\psi(f) = \exp(-\langle f, f\rangle/2) \sum_{n\geq 0} \frac{1}{\sqrt{n!}} f^{\otimes n}. \tag{2.2.3}$$

*In particular, the particle number distribution of the coherent state $\psi(f)$ follows a Poisson distribution with parameter $\langle f, f\rangle$, i.e. the probability of having n particles in $\psi(f)$ is* $\exp(-\langle f, f\rangle)\langle f, f\rangle^n/n!$.

*Proof.* Define the operator $A := i(a^*(f) - a(f))$. As $A$ is symmetric and $D(A) = D(A^*)$ it is self-adjoint. Using the spectral theorem[2] we can write $W(f)$ in the following way

$$W(f) = \exp(-iA) = \int \exp(-i\lambda) dP(\lambda). \tag{2.2.4}$$

[2] See for example Theorem VIII.6. in [21]

Here $P$ denotes the projection-valued measure of $A$. Define the projection $P_f = \chi_{[-2\|f\|,2\|f\|]}(A)$. Then the operator $A$ is bounded on the set $D(f) = P_f \mathscr{F}(\mathcal{H})$. As $\Omega \in D(f)$ we can write

$$\psi(f) = \sum_{n\geq 0} \frac{(-iA)^n}{\sqrt{n!}}\Omega = \exp(-\langle f, f\rangle/2) \sum_{n\geq 0} \frac{(a^*)^n}{n!}\Omega = \exp(-\langle f, f\rangle/2) \sum_{n\geq 0} \frac{1}{\sqrt{n!}} f^{\otimes n}, \tag{2.2.5}$$

where we used $[a(f), a^*(f)] = \langle f, f\rangle$. Let $P_n$ be the projection to the subspace of $n$ particles. Then, using equation (2.2.5), we obtain

$$\langle P_n\psi(f), P_n\psi(f)\rangle = \exp(-\langle f, f\rangle)\frac{\langle f, f\rangle^n}{n!}.$$

Thus, the particle number of $\psi(f)$ follows a Poisson distribution with parameter $\langle f, f\rangle$. □

In the following Lemma we collect some basic properties of the Weyl operators and coherent states.

**Lemma 2.2.2.** *Let $f, g \in \mathcal{H}$.*

1. *$W(f)$ is a unitary operator and*

$$W(f)^* = W(f)^{-1} = W(-f). \tag{2.2.6}$$

2. *The Weyl operator satisfies the relations*

$$W(f)W(g) = W(g)W(f)\exp\big(-2iIm\langle f, g\rangle\big) = W(g+f)\exp\big(-iIm\langle f, g\rangle\big). \tag{2.2.7}$$

   *In particular we have*

$$W(g)\psi(f) = \exp\big(-iIm\langle g, f\rangle\big)\psi(g+f).$$

3. *We have*

$$W^*(f)a(g)W(f) = a(g) + \langle g, f\rangle I, \quad W^*(f)a^*(g)W(f) = a^*(g) + \langle f, g\rangle I. \tag{2.2.8}$$

4. *The coherent states are eigenfunctions of the annihilation operators:*

$$a(g)\psi(f) = \langle g, f\rangle\,\psi(f).$$

5. *The expectation of the number operator $\mathcal{N}$ in the coherent state $\psi(f)$ is*

$$\langle\psi(f), \mathcal{N}\psi(f)\rangle = \langle f, f\rangle,$$

   *also we have the variance*

$$\langle\psi(f), \mathcal{N}^2\psi(f)\rangle - \langle\psi(f), \mathcal{N}\psi(f)\rangle^2 = \langle f, f\rangle.$$

6. *The coherent states are normalized but not orthogonal to each other:*

$$\langle \psi(f), \psi(g) \rangle = \exp\left( -\frac{1}{2} \Big( \|f - g\|^2 - i Im \langle f, g \rangle \Big) \right). \tag{2.2.9}$$

7. *The set of operators $\{W(f) | f \in \mathcal{H}\}$ is irreducible on $\mathscr{F}(\mathcal{H})$: the only bounded operators $\mathcal{B}$ on $\mathscr{F}(\mathcal{H})$ commuting with $W(f)$ for all $f \in \mathscr{F}(\mathcal{H})$ are of the form $B = \lambda I, \lambda \in \mathbb{C}$. In particular the set of coherent states $\{W(f) | f \in \mathcal{H}\}$ is total in $\mathscr{F}(\mathcal{H})$.*

*Proof.* 1. As shown in the proof of Lemma 2.2.1 the operator $A_f := -i(a^*(f) - a(f))$ is self-adjoint. Then the statement follows immediately from Theorem VIII.7 in [21].
2. As in Lemma 2.2.1 we restrict the Hilbert space to a subspace s.t. $A_f$, $A_g$ and $A_{f+g}$ are bounded and s.t. the vacuum $\Omega$ is contained in this subspace. Then the operators $W(g)$, $W(f)$, $W(f+g)$ can be written in a power series and the properties in (2.2.7) can be computed. We leave the details to the reader.
3. Theorem VIII.7 in [21] implies that $\frac{\mathrm{d}}{\mathrm{d}t} W(tf) = \frac{\mathrm{d}}{\mathrm{d}t} \exp(itA_f)$ exists for any $f \in \mathcal{H}$ and any $t \in \mathbb{R}$. Moreover it says that

$$\frac{\mathrm{d}}{\mathrm{d}t'} W(t'f)\Big|_{t'=t} = (a^*(f) - a(f)) W(tf) \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t'} W^*(t'f)\Big|_{t'=t} = W^*(tf)(a(f) - a^*(f)).$$

Thus we can compute

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t'} W^*(t'f) a(g) W(t'f)\Big|_{t'=t} &= W^*(tf)\Big( (a(f) - a^*(f)) a(g) + a(g)(a^*(f) - a(f)) \Big) W(tf) \\ &= W^*(tf)[a(g), a^*(f)] W(tf) = \langle g, f \rangle I. \end{aligned}$$

By the fundamental theorem of calculus (which can also be justified by Theorem VIII.7 in [21]) we obtain

$$W^*(f) a(g) W(f) - a(g) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} W^*(tf) a(g) W(tf) dt = \langle g, f \rangle I.$$

The corresponding statement for $a^*(g)$ follows similarly.
4. Statements (2.2.6) and (2.2.8) imply

$$a(g)\psi(f) = a(g) W(f)\Omega = W(f)\Big( a(g) + \langle g, f \rangle I \Big)\Omega = \langle g, f \rangle \psi(f).$$

5. This statement immediately follows from Lemma 2.2.1.
6. Using statements (2.2.6), (2.2.7) and Lemma 2.2.1 we compute

$$\begin{aligned} \langle \psi(f), \psi(g) \rangle &= \langle \Omega, W^*(f) W(g) \Omega \rangle = \langle \Omega, W(g - f)\Omega \rangle \exp\left( i \mathrm{Im}(f, g) \right) \\ &= \exp\left( -\frac{1}{2} \Big( \|f - g\|^2 - i \mathrm{Im} \langle f, g \rangle \Big) \right). \end{aligned}$$

7. As $B$ commutes with any $\psi(f)$ with $f \in \mathcal{H}$, it commutes in particular with any $a(f)$ and any $a^*(f)$. Thus, $B$ commutes with the number operator $\mathcal{N}$. Let $\{e_i\}_{i=1}^{\infty}$ be an orthonormal basis of $\mathcal{H}$ and denote $a_i = a(e_i)$. Then the vectors $\psi_{k_1,\dots,k_n} = (k_1! \dots k_n!)^{-1/2} (a_1^*)^{k_1} \dots (a_n^*)^{k_n} \Omega$ with the obvious index set are an

orthonormal basis of $\mathscr{F}(\mathcal{H})$. As $B$ commutes with all $a_i$ and $a_i^*$ we have $\langle \psi_{k_1,...,k_n}, B\psi_{j_1,...,j_m}\rangle = 0$ if the sets $\{k_1, ..., k_n\}$, $\{j_1, ..., j_m\}$ are different. Using the canoncial commutation relations we have

$$\langle \psi_{k_1,...,k_n}, B\psi_{k_1,...,k_n}\rangle = (k_1!...k_n!)^{-1} \langle \Omega, Ba_{i_1}...a_{i_n}a_{i_1}^*...a_{i_n}^*\Omega\rangle = \langle \Omega, B\Omega\rangle .$$

Thus $B = \langle \Omega, B\Omega\rangle I$. □

As an example we consider again a bosonic gas in the box represented by $\mathscr{F}(L^2(\Lambda_L))$. On the condensate space $\mathcal{F}_0$, i.e. the Fock space of span$(L^{-2/3})$, we define the Weyl operators

$$W_z := \exp[za_0^* - \overline{z}a_0], \quad \text{where } z \in \mathbb{C}. \tag{2.2.10}$$

The corresponding coherent states are

$$|z\rangle := W_z |\Omega\rangle , \quad \text{where } z \in \mathbb{C}. \tag{2.2.11}$$

Due to Lemma 2.2.2 we have the following identities

$$W_z^* a_0 W_z = a_0 + z, \quad W_z^* a_0^* W_z = a_0^* + \overline{z}. \tag{2.2.12}$$

Moreover, the last statement of Lemma 2.2.2 implies that we have

$$\int_{\mathbb{C}} |z\rangle \langle z| \, dz = 1_{\mathscr{F}_0}, \tag{2.2.13}$$

where for $z = x + iy$ we have the measure $dz = \pi^{-1}dxdy$.

## 2.3 Quantum Statistical Mechanics

The content of this section is mainly taken from chapter 2 in [24] and chapter 8 in [14].
For simplicity we only consider the bosonic case. In quantum statistical mechanics physical states are expressed by the following operators:

**Definition 2.3.1.** An operator $\Gamma \in \mathcal{B}(\mathscr{F}(\mathcal{H}))$ is called a state if it is nonnegative (denoted by $\Gamma \geq 0$) and if $\mathrm{Tr}[\Gamma] = 1$. We denote the set of states in $\mathcal{B}(\mathscr{F}(\mathcal{H}))$ by $\mathscr{S}$.

Due to the polarization identity any bounded, positive operator on a complex Hilbert space is self-adjoint.[3] Because trace-class implies boundedness and even compactness we see that all states are in fact self-adjoint. By the Hilbert-Schmidt Theorem[4] we find a complete orthonormal basis $\{\psi_\alpha\}_{\alpha=1}^\infty$ of eigenvectors of $\Gamma$ and we can write the state in the form

$$\Gamma = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\psi_\alpha\rangle \langle \psi_\alpha| . \tag{2.3.1}$$

[3] See section VI.4 in [21]
[4] See Theorem VI.16 in [21]

Here $\langle\psi_\alpha| \in \mathscr{F}(\mathcal{H})^*$ is the, to $\psi_\alpha$ corresponding, element of the dual Fock space $\mathscr{F}(\mathcal{H})^*$ (correspondence by the Riesz representation theorem). Then the action of $|\psi_\alpha\rangle\langle\psi_\alpha| \in \mathscr{F}(\mathcal{H}) \otimes \mathscr{F}(\mathcal{H})^*$ on some $\phi \in \mathscr{F}(\mathcal{H})$ is interpreted as $|\psi_\alpha\rangle\langle\psi_\alpha|\,\phi = \langle\psi_\alpha, \phi\rangle\,\psi_\alpha$.
Moreover, applying functional calculus[5] we can define $f(\Gamma)$ in the natural way as

$$f(\Gamma) := \sum_{\alpha=1}^{\infty} f(\lambda_\alpha)\,|\psi_\alpha\rangle\langle\psi_\alpha|\,,$$

for any $f \in \mathscr{B}(\mathbb{R})$.
We will call a state pure if the operator $\Gamma$ is a one-dimensional projection. To measure how far from being pure a state is we introduce the von Neumann entropy, which we will simply call the entropy from now on.

**Definition 2.3.2.** The entropy of a state as in definition 2.3.1 is given by

$$S(\Gamma) = -\operatorname{Tr}[\Gamma \ln(\Gamma)], \tag{2.3.2}$$

which is possibly $+\infty$. We use the convention $t\ln(t) = 0$ if $t = 0$.

It is easy to see that the entropy vanishes if and only if the state is pure.
An observable $o$ in quantum mechanics is represented by a self-adjoint operator $O$ acting on the Hilbert space. In quantum statistical mechanics, if the state of the system is represented by $\Gamma \in \mathscr{S}$ then the expectation of the observable $o$ is given by

$$\mathbb{E}[o] = \operatorname{Tr}[O\Gamma]. \tag{2.3.3}$$

Let us consider a system with a fixed number of particles $N$, fixed temperature $T \geq 0$ and fixed volume $V$. This is called the canonical setting. Let $H$ be the Hamiltonian of the system and define $\beta := T^{-1}$. At zero temperature we assume that the system is stable, which means

$$\inf_{\Gamma\in\mathscr{S}_N} \operatorname{Tr}[H\Gamma] > -\infty \iff \inf\sigma(H) > -\infty.$$

Here $\mathscr{S}_N$ denotes the set of states with $N$ particles and $\sigma(H)$ denotes the spectrum of $H$. If a state attains the infimum it is called a ground state, which is always a pure state. The value of the infimum is called the ground state energy. For temperatures $T \geq 0$ we define the free energy of the system.

**Definition 2.3.3.** The Gibbs free energy functional of a stable $N$-particle system in a volume $V$ with Hamiltonian $H$ and temperature $T \geq 0$ is defined by

$$\mathcal{F}(\Gamma) = \operatorname{Tr}[H\Gamma] - TS(\Gamma), \tag{2.3.4}$$

where $\Gamma \in \mathscr{S}_N$. The canonical free energy of the system then is

$$F(N, V, T) = \inf_{\Gamma\in\mathscr{S}_N} \mathcal{F}(\Gamma). \tag{2.3.5}$$

[5] See Theorem VII.2 in [21]

**Remark 2.3.1.** The free energy can also be minus infinity. For example assume that $\dim(\ker(H))$ is infinite. Then we can find an orthonormal set $\{\psi_n\}_{n=1}^{\infty}$ of vectors of $\ker(H)$. Define the sequence of states

$$\Gamma_k := \sum_{n=1}^{\infty} \lambda_{n,k} |\psi_n\rangle \langle\psi_n|$$

with $\lambda_{n,k} = n^{-1-1/k} C_k^{-1}$ where $C_k = \sum_{n=1}^{\infty} n^{-1-1/k}$. Then we have for $T > 0$

$$\mathcal{F}(\Gamma_k) = T \sum_{n=1}^{\infty} \lambda_{n,k} \ln\left(\lambda_{n,k}\right) = -T \frac{(1+1/k)}{C_k} \sum_{n=1}^{\infty} \frac{\ln(n)}{n^{1+1/k}} - T \frac{\ln(C_k)}{C_k} \sum_{n=1}^{\infty} \frac{1}{n^{1+1/k}} \leq -T \ln(C_k) \xrightarrow{k\to\infty} -\infty.$$

In this case we just define the free energy to be minus infinity. On the contrary if the ground state energy is finite then the free energy is bounded from above by the ground state energy. This follows from the following Lemma:

**Lemma 2.3.1.** *$F(N, V, T)$ is a decreasing function with respect to $T$. Moreover, the free energy at zero temperature is equal to the ground state energy.*

*Proof.* Note that $t \ln(t) \leq 0$ for $0 \leq t \leq 1$. Thus $S(\Gamma) \geq 0$ for any state $\Gamma$. Let $T' \geq T$ and let $\{\Gamma_n\}_{n=1}^{\infty}$ be a minimizing sequence of states for $F(N, V, T)$. Then we have by the variational principle

$$F(N, V, T) = \lim_{n\to\infty} \Big( \mathrm{Tr}[H\Gamma_n] - TS(\Gamma_n) \Big) \geq \lim_{n\to\infty} \Big( \mathrm{Tr}[H\Gamma_n] - T'S(\Gamma_n) \Big) \geq F(N, V, T'). \tag{2.3.6}$$

It is obvious that the free energy at zero temperature equals the ground state energy. □

If the free energy is finite we have a unique minimizer of the canonical free energy functional (2.3.4). We call this minimizer the Gibbs state.

**Lemma 2.3.2.** *Let $H$ be s.t. the system is stable at $T = 0$. Fix $T \geq 0$ s.t. the free energy is finite. Then the unique minimizer of the Gibbs free energy functional* (2.3.4) *is given by*

$$\Gamma_{\mathrm{G}} = \frac{\exp(-T^{-1}H)}{\mathrm{Tr}[\exp(-T^{-1}H)]}. \tag{2.3.7}$$

*Furthermore, the canonical free energy can be written as*

$$F(N, V, T) = -T \ln\Big( \mathrm{Tr}[\exp(-T^{-1}H)] \Big). \tag{2.3.8}$$

*Proof.* As the system is stable at zero temperature we have by Lemma 2.3.1 that the free energy is bounded from above for any $T \geq 0$. Furthermore, by assumption we have that $F(N, V, T) > -\infty$. Thus, $F(N, V, T)$ is finite. Define the function $\phi(x) = x \ln(x)$. Note that

$$\begin{aligned} \phi'(\Gamma_{\mathrm{G}}) &= -T^{-1}H - \ln\Big( \mathrm{Tr}[\exp(-T^{-1}H)] \Big) + 1 \\ \implies \quad H &= -T\phi'(\Gamma_{\mathrm{G}}) - T \ln\Big( \mathrm{Tr}[\exp(-T^{-1}H)] \Big) + T. \end{aligned}$$

Thus we can write for a state $\Gamma$

$$\begin{aligned}\mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_G) &= \mathrm{Tr}\,[H(\Gamma - \Gamma_G)] + T\,\mathrm{Tr}\,[\phi(\Gamma)] - T\,\mathrm{Tr}\,[\phi(\Gamma_G)] \\ &= T\,\mathrm{Tr}\,[\phi(\Gamma) - \phi(\Gamma_G) - \phi'(\Gamma_G)(\Gamma - \Gamma_G)]. \end{aligned} \tag{2.3.9}$$

Let $\{\lambda_\alpha\}_{\alpha=1}^\infty$ resp. $\{\nu_\beta\}_{\beta=1}^\infty$ be the eigenvalues of $\Gamma_G$ resp. of $\Gamma$ and let $\{f_\alpha\}_{\alpha=1}^\infty$ resp. $\{g_\beta\}_{\beta=1}^\infty$ be a corresponding orthonormal basis of eigenvectors. Then with a similar argument as used in the proof of Klein's inequality[6] we have

$$\mathrm{Tr}\,[\phi(\Gamma) - \phi(\Gamma_G) - \phi'(\Gamma_G)(\Gamma - \Gamma_G)] = \sum_{\alpha,\beta=1}^{\infty} |\langle f_\alpha, g_\beta\rangle|^2 \Big(\phi(\nu_\beta) - \phi(\lambda_\alpha) - \phi'(\lambda_\alpha)(\nu_\beta - \lambda_\alpha)\Big) \geq 0, \tag{2.3.10}$$

where we used that the function $\phi$ is convex. As $\phi$ is even strictly convex we have equality in (2.3.10) if and only if for any $1 \leq \alpha, \beta < \infty$ we have $\langle f_\alpha, g_\beta\rangle = 0$ or $\lambda_\alpha = \nu_\beta$. But this would imply that any $f_\alpha$ is an eigenvector of $\Gamma$ with eigenvalue $\lambda_\alpha$ which yields $\Gamma = \Gamma_G$. Thus, considering (2.3.9) and (2.3.10) we obtain for all states $\Gamma$:

$$\mathcal{F}(\Gamma) \geq \mathcal{F}(\Gamma_G), \quad \text{with equality iff } \Gamma = \Gamma_G.$$

This proves that the state $\Gamma_G$ is the unique minimizer of the Gibbs free energy functional. The formula (2.3.8) for the free energy is obtained by calculating $\mathcal{F}(\Gamma_G)$. □

The result (2.3.8) suggest that it is reasonable to describe the system with the following quantity:

**Definition 2.3.4.** The canonical partition function corresponding to the Gibbs state (2.3.7) is defined as

$$Z_c(N, V, T) = \mathrm{Tr}\,[\exp(-T^{-1}H)].$$

Often we want to analyze open systems or we simply do not know how many particles the system contains. In this case it is unreasonable to fix the particle number $N$. Therefore a new quantity, the chemical potential $\mu$, takes its place. It can be thought of the average amount of energy needed to remove one particle from the system. This is described by $H \mapsto H - \mu\mathcal{N}$ where $H$ is the second quantization of the Hamiltonian. For fixed $T$, $V$, $\mu$ the system is described by the grand canonical ensemble. The analogue to the free energy in the canonical ensemble is the grand potential $\Phi$ in the grand canonical ensemble. It is given by

$$\Phi(\mu, V, T) = \inf_{\Gamma \in \mathscr{S}} \Big\{ \mathrm{Tr}\,[(H - \mu\mathcal{N})\Gamma] - TS(\Gamma) \Big\}, \tag{2.3.11}$$

where the set of states $\mathscr{S}$ is defined by 2.3.1. We can prove the same result as in Lemma 2.3.2 for the grand canonical ensemble:

$$\Phi(\mu, V, T) = -T \ln\Big(Z_{gc}(\mu, V, T)\Big), \tag{2.3.12}$$

[6] See subsection 2.1.4 in [28]

where

$$Z_{\mathrm{gc}}(\mu, V, T) = \mathrm{Tr}\left[\exp\left(-T^{-1}(H - \mu\mathcal{N})\right)\right] = \sum_{N=0}^{\infty} z^N Z_{\mathrm{c}}(N, V, T) \tag{2.3.13}$$

is the grand canonical partition function. Here $z = \exp(T^{-1}\mu)$ is called the fugacity. Furthermore, the grand canonical Gibbs state $\Gamma_{\mathrm{G}}$ is defined as in (2.3.7) except exchanging $H$ by $H - \mu\mathcal{N}$. We can define a grand canonical version of the free energy by

$$F^{\mathrm{gc}}(N, V, T) = \inf_{\Gamma \in \mathscr{S}_N^{\mathrm{gc}}} \Big\{ \mathrm{Tr}\left[H\Gamma\right] - T^{-1} S(\Gamma) \Big\}, \tag{2.3.14}$$

where we choose to minimize over

$$\mathscr{S}_N^{\mathrm{gc}} := \Big\{ \Gamma \in \mathcal{B}(\mathscr{F}(L^2(\Lambda_L))) \Big| \Gamma \geq 0, \mathrm{Tr}\left[\Gamma\right] = 1, \mathrm{Tr}\left[\mathcal{N}\Gamma\right] = N, \mathrm{Tr}\left[H\Gamma\right] < \infty \Big\}, \tag{2.3.15}$$

the set of all states with expected number of particles $N$. If we choose the chemical potential $\mu$ s.t. we have for the Gibbs State $\mathrm{Tr}\left[\mathcal{N}\Gamma_{\mathrm{G}}\right] = N$ then we have the useful relation

$$F^{\mathrm{gc}}(N, V, T) = \Phi(\mu, V, T) + \mu N. \tag{2.3.16}$$

Not only the grand potential can be calculated using the grand partition function. For example we can also compute the expected number of particles in the Gibbs state:

$$N = z\frac{\partial}{\partial z} \ln\Big(Z_{\mathrm{gc}}(\mu, V, T)\Big). \tag{2.3.17}$$

Or the expected number of particles with energy $E_\alpha$ in $\Gamma_G$:

$$n_\alpha = -T\frac{\partial}{\partial E_\alpha} \ln\Big(Z_{\mathrm{gc}}(\mu, V, T)\Big). \tag{2.3.18}$$

## 2.4 The Ideal Bose Gas

In this section we analyze the ideal Bose Gas on the flat torus $\Lambda_L$ in a grand canonical setting. This is one of the few example where we are able to compute explicit formulas for the partition function and therefore for the free energy of the system. We will heavily base our calculations in Chapter 4 on the results obtained for the ideal Bose gas. If not stated otherwise, the material for this section is taken from Chapter 8 and 12 in [14]. For the treatement of the BEC transition we also consulted [9] and [18].
As derived in section 2.1, the Hamiltonian of the ideal Bose gas in the box $\Lambda_L$ takes the second quantized form

$$d\Gamma(-\Delta) = \sum_{p \in \Lambda_L^*} p^2 a_p^* a_p,$$

where $\Lambda_L^* := (2\pi/L)\mathbb{Z}^3$. According to the grand canonical version of Lemma 2.3.2 the Gibbs state is given by

$$\Gamma_{\mathrm{G}} = \frac{\exp(-T^{-1}d\Gamma(-\Delta-\mu))}{\mathrm{Tr}[\exp(-T^{-1}d\Gamma(-\Delta-\mu))]}. \tag{2.4.1}$$

Let us calculate the grand canonical partition function of the ideal Bose gas. For convenience we index the elements of the set $\{p \in \Lambda_L^*\}$ and denote it by $\{p_j\}_{j=1}^{\infty}$. Moreover, we define the set $S_N = \{(n_1, n_2, ...) \in \mathbb{N}^{\mathbb{N}} \big| \sum_{j=1}^{\infty} n_j = N\}$ for any $N \in \mathbb{N}$. Then we can write for the grand canonical partition function

$$\begin{aligned} Z_{\mathrm{gc}}(z,V,T) &= \sum_{N=0}^{\infty} z^N Z_c(N,V,T) = \sum_{N=0}^{\infty} z^N \sum_{n\in S_N} \exp\left(-T^{-1}\sum_{j=1}^{\infty} p_j^2 n_j\right) \\ &= \sum_{N=0}^{\infty}\sum_{n\in S_N}\prod_{j=1}^{\infty}\left(z\exp\left(-T^{-1}p_j^2\right)\right)^{n_j} \\ &= \prod_{j=1}^{\infty}\left[\sum_{k=0}^{\infty}\left(z\exp\left(-T^{-1}p_j^2\right)\right)^k\right] \\ &= \prod_{p\in\Lambda_L^*}\frac{1}{1-\exp(-T^{-1}(p^2-\mu))} \end{aligned} \tag{2.4.2}$$

Thus, using (2.3.17), the expected particle number of the Gibbs state is given by the equation

$$N = \sum_{p\in\Lambda_L^*}\frac{1}{\exp(\beta(p^2-\mu))-1}, \tag{2.4.3}$$

where we denote $\beta = T^{-1}$. Moreover, with (2.3.18), the average number of particles $\langle n_p\rangle$ with momentum $p \in \Lambda_L^*$ is given by

$$\langle n_p\rangle = \frac{1}{e^{\beta(p^2-\mu)}-1}. \tag{2.4.4}$$

More generally, we can write the matrix elements of the one-particle density matrix explicitly as

$$\hat{\gamma}_0(p,q) = \mathrm{Tr}[a_q^* a_p \Gamma_0] = \delta_{p,q}\langle n_p\rangle. \tag{2.4.5}$$

This can be seen as follows: Because the Fourier basis functions are eigenfunctions of the Laplacian we can write by functional calculus

$$\Gamma_{\mathrm{G}} = \sum_{\alpha=1}^{\infty}\lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|,$$

where any $\psi_\alpha$ is a $N_\alpha$-fold symmetric tensor product of Fourier basis elements. Therefore, we can write the trace in (2.4.5) as

$$\mathrm{Tr}[a_q^* a_p \Gamma_0] = \sum_{\alpha=1}^{\infty}\lambda_\alpha\langle a_q\psi_\alpha, a_p\psi_\alpha\rangle.$$

It is easy to see that $\langle a_q\psi_\alpha, a_p\psi_\alpha\rangle = \delta_{p,q}N_\alpha(p)$, where $N_\alpha(p)$ is the number of particles in $\psi_\alpha$ with momentum $p$. Thus,

$$\mathrm{Tr}[a_q^* a_p \Gamma_0] = \sum_{\alpha=1}^{\infty} \lambda_\alpha \delta_{p,q} N_\alpha(p) = \delta_{p,q} \langle n_p \rangle .$$

From equation (2.4.5) we see that the one-particle density matrix of the ideal Bose gas Gibbs state is diagonal in the Fourier basis. From now on we denote its diagonal elements by $\hat{\gamma}_0(p)$.
To compute the general $n$-particle density matrix of $\Gamma_\mathrm{G}$ we can apply the Wick theorem. We will state it here for the specific case of the ideal Bose gas. For the proof of the Wick theorem for the general case of quasi-free pure states see Theorem 10.2 in [24].

**Theorem 2.4.1.** *Let $\Gamma_\mathrm{G}$ be the state defined in* (2.4.1)*. Then its n-particle density matrix satisfies*

$$\mathrm{Tr}[a_{p_1}^* ... a_{p_n}^* a_{q_1} ... a_{q_n} \Gamma_\mathrm{G}] = \sum_{\sigma \in S_n} \prod_{k=1}^{n} \mathrm{Tr}[a_{p_k}^* a_{q_{\sigma(k)}} \Gamma_\mathrm{G}], \tag{2.4.6}$$

*where $\{p_k\}_{k=1}^n, \{q_k\}_{k=1}^n \subset \Lambda_L^*$ and $S_n$ denotes the group of permutations of n elements.*

The following propostion from [10, Proposition A.1.] states that the canonical free energy of the ideal Bose gas is a convex function with respect to the particle number $N$. As the proof is rather long we omit it here. It can be found in [26]. To simplify the notation we denote by $F_0(N)$ the canonical free energy of the Gibbs state of the ideal gas with $N$ particles. Moreover, by $F_0^{\mathrm{gc}}(\mu)$ we denote the corresponding grand canonical version of the free energy.

**Proposition 2.4.1.** *The map $N \mapsto F_0(N)$ is convex, i.e., $F_0(N+1) + F_0(N-1) \geq 2F_0(N)$ holds for all $N \geq 1$.*

We can relate the grand canonical to the canonical free energy of the ideal Bose gas. The following Corollary from [10, Corollary A.1.] quantifies in what sense we can compare them.

**Corollary 2.4.1.** *Assume $\mu$ is such that $\mathrm{Tr}[\mathcal{N}\Gamma_G] = N$. Then*

$$F_0(N) \geq F_0^{\mathrm{gc}}(\mu) \geq F_0(N) - T\ln(1+N) - T. \tag{2.4.7}$$

*Proof.* Define $\lambda := \{\lambda_{n,\mu}\}_{n\in\mathbb{N}}$ where $\lambda_{n,\mu} = Z(n)\exp(T^{-1}\mu n)/Z_{\mathrm{gc}}(\mu)$. Due to proposition 2.4.1 we have that the map $N \mapsto F_0(N)$ is convex. Thus $\sum_{n=0}^{\infty} \lambda_{n,\mu} F_0(n) \geq F_0(N)$. Note that we have $F_0^{\mathrm{gc}} = \sum_{n=0}^{\infty} \lambda_{n,\mu} F_0(n) - TS(\lambda)$. Denote by $\mathcal{M}$ the set of all real, nonnegative sequences $w = \{w_n\}_{n=0}^{\infty}$ with the properties $\sum_{n=0}^{\infty} w_n = 1$ and $\sum_{n=0}^{\infty} n w_n = N$. By definition $S(\lambda) \leq \sup_{w\in\mathcal{M}} S(w)$. The supremum on the r.h.s can be computed explicitly and equals $\ln(1+N) + N\ln\left((1+N)/N\right)$. Since $N\ln\left((1+N)/N\right) \leq 1$ this proves the lower bound of $F_0^{\mathrm{gc}}(\mu)$. The upper bound follows from the Gibbs variational principle. □

In the large particle number limit the ideal Bose gas displays a BEC phase transition. By equation (2.4.3) the expected number of particles is given by

$$N = \sum_{p \in \Lambda_L^* \setminus \{0\}} \frac{1}{z^{-1} \exp(\beta p^2) - 1} + \frac{1}{z^{-1} - 1}, \tag{2.4.8}$$

which clearly implies $\mu < 0$ or equivalently $z \in [0, 1)$. In the thermodynamic limit the first term on the r.h.s of (2.4.8) can be written as an integral which yields the equation

$$\varrho = 4\pi \int_0^\infty dp p^2 \frac{1}{z^{-1} \exp(\beta p^2) - 1} + \varrho_0. \tag{2.4.9}$$

Here we took the limit $N, L \to \infty$ while keeping $\varrho = N/L^3$ fixed. Moreover $\varrho_0 = \lim_{L\to\infty} L^{-3} z/(1-z)$ where the dependence between $L$ and $\mu$ is determined by $N = L^3 \varrho$. The crucial point is that the first term on the r.h.s of (2.4.8) takes the finite value $\varrho_c(\beta)$ for $z \to 1$. Here

$$\varrho_c(\beta) = (2\pi\beta)^{-3/2} g_{3/2}(1), \quad \text{where} \quad g_{3/2}(1) = \sum_{k=1}^{\infty} \frac{1}{k^{3/2}} = \zeta(3/2). \tag{2.4.10}$$

Thus for $\varrho > \varrho_c$ we obtain the equation

$$\varrho = \varrho_c(\beta) + \varrho_0. \tag{2.4.11}$$

Rearranging equation (2.4.11) gives the relation

$$\frac{N_0}{N} \simeq \left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right]_+ \quad \text{with} \quad T_c = 4\pi \left(\frac{\varrho}{\zeta(3/2)}\right)^{2/3}. \tag{2.4.12}$$

Here we denote $[x]_+ = \max\{x, 0\}$. $T_c$ is called the critical temperature. Thus we see that for temperatures lower than the critical temperature we expect a positive fraction of particles in the condensate.

**Remark 2.4.1.** In formula (2.4.12) we see that $\beta_c \sim \varrho^{-2/3}$. Thus to investigate a Bose gas around the critical temperature it is reasonable to keep $\beta\varrho^{2/3}$ fixed. This is exactly what is considered in the Gross-Pitaevskii limit.

## 2.5 The Scattering Equation

As already discussed in the introduction, the interaction of two bosonic particles in dilute quantum gases is described by the zero energy scattering equation

$$\left[-\Delta + \frac{1}{2}V\right]\phi = 0. \tag{2.5.1}$$

where $V$ is assumed to be nonnegative, spherically symmetric and compactly supported on $B_{R_0} := \{x : 0 < |x| < R_0\}$. Note that $V$ nonnegative implies that for any $\phi \in H^1$ (the space of $L^2(\mathbb{R}^3)$ functions with $L^2(\mathbb{R}^3)$ derivatives) we obviously have

$$\int_{\mathbb{R}^3} \left( \left|\nabla\phi(x)\right|^2 + \frac{1}{2}V(x)\left|\phi(x)\right|^2 \right) dx \geq 0. \tag{2.5.2}$$

The following theorem taken from [18, Appendix C] gives the existence of a solution of the scattering equation (2.5.1) confined to a ball of radius $R$. Moreover, the theorem describes the asymptotic behaviour of this solution which gives us the definition of the scattering length $a$.
It should be noted that we do not actually apply this theorem in our proof of the main result. For this we need an adjusted version which is presented in the second part of this section. We decided to state and prove the following theorem because we think it gives us a better intuition about the scattering process.

**Theorem 2.5.1.** *Let $R > R_0$ and denote by $S_R$ the sphere $\{x : |x| = R\}$. For $f \in H^1(B_R)$ we set*

$$\mathcal{E}_R(\phi) = \int_{B_R} \left( \left|\nabla\phi(x)\right|^2 + \frac{1}{2}V(x)\left|\phi(x)\right|^2 \right) dx. \tag{2.5.3}$$

*Then, in the subclass of functions such that $\phi(x) = 1$ for all $x \in S_R$, there is a unique function $\phi_0$ that minimizes $\mathcal{E}_R(\phi)$. This function is nonnegative and spherically symmetric, i.e. $\phi_0(x) = f_0(|x|)$ with a nonnegative function $f_0$ on the interval $(0, R]$, and it satisfies the equation*

$$\left[ -\Delta + \frac{1}{2}V \right] \phi_0 = 0 \tag{2.5.4}$$

*in the sense of distribution on $B_R$, with boundary condition $f_0(R) = 1$. Furthermore we have the following:*

1. *For $R_0 < r < R$ we have*

$$f_0(r) = f_0^{asymp}(r) = \frac{1 - ar^{-1}}{1 - aR^{-1}} \tag{2.5.5}$$

   *for some number $a$ called the scattering length of $V$.*

2. *We have $f_0(r) \geq f_0^{asymp}(r)$ for $0 < r < R_0$.*

3. *$f_0(r)$ is a monotonically nondecreasing function of $r$.*

4. *If $V(r) \geq \tilde{V}(r)$ for all $r$ then the corresponding minimizers satisfy $f_0(r) \leq \tilde{f}_0(r)$ for all $r < R$. Hence, $a > \tilde{a} \geq 0$.*

5. *The minimum value of $\mathcal{E}_R(\phi_0)$ is*

$$E = 4\pi a[(1 - aR^{-1})]^{-1}. \tag{2.5.6}$$

**Remarks 2.5.1.** 1. Condition $V \geq 0$ can be relaxed to $V_- \in L^{3/2}(\mathbb{R}^3)$ such that (2.5.2) still holds. Here $V_-$ is the negative part of the potential $V$. But then points 2., 3. and 4. do not necessarily

hold. The condition $V_- \in L^{3/2}(\mathbb{R}^3)$ ensures that the functional (2.5.3) is bounded from below.[7] The condition (2.5.2) ensures that there are no bound states.

2. By the variational principle $E$ defined in (2.5.6) is a lower bound for the functional (2.5.3). Thus, inserting the test function $\psi = 1$ into (2.5.3) gives us a connection between the scattering length and the potential:

$$4\pi a[(1 - aR^{-1})]^{-1} \leq \mathcal{E}_R(1) = \frac{1}{2}\int_{\mathbb{R}^3} V(x)dx$$
$$\implies 8\pi a \leq \int_{\mathbb{R}^3} V dx. \tag{2.5.7}$$

*Proof.* Given any $\phi \in H^1$ we can replace it by the square root of the spherical average of $|\phi|^2$. This preserves the boundary condition at $|x| = R$, while the $V$ term in (2.5.3) is unchanged. It also lowers the gradient term in (2.5.3) because the map $\varrho \mapsto \int (\nabla \sqrt{\varrho})^2$ is convex.[8] Indeed, there is a strict decrease unless $\phi$ is already spherically symmetric and nonnegative.
Thus, without loss of generality, we may consider only nonnegative, spherically symmetric functions. If we substitute for $\phi$ a harmonic function on the annulus $\mathcal{A} = \{x : R_0 \leq |x| \leq R\}$ that agrees with $\phi$ at $|x| = R_0$ and $|x| = R$ we will lower $\mathcal{E}_R$ unless $\phi$ is already harmonic on $\mathcal{A}$. Thus we can assume on $\mathcal{A} = \{x : R_0 \leq |x| \leq R\}$ that

$$0 = \Delta\phi(x) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{1}{r^2}\frac{\partial\phi(r)}{\partial r}\right).$$

Solving this differential equation with boundary conditions $\phi(R) = 1$ and $\phi(R_0) = \phi_0(R_0)$, where $\phi_0$ is a minimizer on $B_{R_0}$, we see that there exists some $a$ such that (2.5.5) is true.
Because $V \geq 0$ we have that $\mathcal{E}_R(\phi)$ is bounded below. Take a minimizing sequence $\phi^j$ for $\mathcal{E}_R$. Moreover, let $h$ be a smooth function on $\mathbb{R}_+$ with $h(r) = 1$ for $r < R + 1$ and $h(r) = 0$ for $r > 2R + 1$. Then the function $\hat{\phi}^j(x) = \phi^j(x)$ for $|x| \leq R$ and $\hat{\phi}^j(x) = h(|x|)$ for $|x| > R$ is a legitimate variational function for the $L^2(\mathbb{R}^3)$ problem in (2.5.2). As $V$ is positive we see that the kinetic energy $T^j = \int |\nabla\phi^j|^2$ and $\int |\phi^j|^2$ are bounded. By the Banach-Alaoglu Theorem[9] we find a subsequence of the $\hat{\phi}^j$ that converges weakly in $H^1$ to some spherically symmetric $\hat{\phi}_0 = \hat{f}_0(|x|)$. Correspondingly, $\phi^j(x)$ converges weakly in $H^1(B_R)$ to $\phi_0(x) = f_0(|x|)$. The important point is that the term $\int V|\phi^j|^2$ is weakly lower continuous.[10] We also note that $f_0(R) = 1$ since the functions $\hat{\phi}^j$ are identically equal to 1 for $R < |x| < R + 1$ and the limit $\hat{\phi}_0$ is continuous away from the origin since it is spherically symmetric and in $H^1$.
Thus the limit function $\phi_0$ is a minimizer for $\mathcal{E}(\phi)$ under the condition $\phi = 1$ on $S_R$. Since it is a minimizer, it must be harmonic in $\mathcal{A}$, so (2.5.5) is true. Equation (2.5.4) is standard and is obtained by replacing $\phi_0$ by $\phi_0 + \delta\psi$, where $\psi$ is any infinitely differentiable function that is zero for $|x| \geq R$. The first variation in $\delta$ gives (2.5.4). [11]
The uniqueness of the minimizer can be proved in two ways. One way is to note that if $\phi_0 \neq \psi_0$ are

[7] See [16], section 11.3
[8] See Theorem 7.8 in [16]
[9] See Theorem IV.21 in [21]
[10] See Theorem 11.4 in [16]
[11] See the proof of Theorem 11.5 in [16]

two minimizers then, by the convexity noted above, $\mathcal{E}_R\Big((\phi_0^2+\psi_0^2)^{1/2}\Big) < \mathcal{E}_R(\phi_0)+\mathcal{E}_R(\psi_0)$. The second way is to notice that all minimizers satisfy (2.5.4), which is a linear, ordinary differential equation for $f_0$ on $(0,R)$ since all minimizers are spherically symmetric, as we noted. But the solution of such equations, given the value at the end points, is unique.
2. For $r \geq R$ we extend the solution by setting $f_0(r) = f_0^{asymp}(r)$. As we have $V \geq 0$ and already showed $\phi_0 \geq 0$ we have $\Delta\phi_0 \geq 0$ using equation (2.5.4). Thus by Theorem 9.3 in [16] $\phi_0$ is subharmonic. Set $h_\varepsilon(r) = f_0(r) - (1+\varepsilon)f_0^{asymp}(r)$ with $\varepsilon > 0$ small. Obviously, $x \mapsto h_\varepsilon(|x|)$ is subharmonic on the open set $\{x : 0 < |x| < \infty\}$ because $f_0^{asymp}(|x|)$ is harmonic there. Clearly, $h_\varepsilon \to -\infty$ as $r \to \infty$ and $h_\varepsilon(R) = -\varepsilon$. Suppose that the inequality in 2. is false at some radius $\varrho < R$ and that $h_0(\varrho) = -c < 0$. In the annulus $\varrho < r < \infty$, $h_\varepsilon(r)$ has its maximum on the boundary, i.e., either at $\varrho$ or at $\infty$ (since $h(|x|)$ is subharmonic in $x$).[12] By choosing $\varepsilon$ sufficiently small and positive we can have that $h_\varepsilon < -2\varepsilon$ and this contradicts the fact that the maximum (which is at least $-\varepsilon$) is on the boundary.
3. By subharmonicity the maximum of $f_0$ in $(0,r)$ occurs on the boundary, i.e., $f_0(r) \geq f_0(r')$ for any $r' < r$.
4. We study the function $g = f_0 - \tilde{f}_0$. Since $f_0$ and $\tilde{f}_0$ are continuous, the falsity of 4. implies the existence of some open subset, $\Omega \subset B_R$ on which $g(|x|) > 0$. On $\Omega$ we have that $g(|x|) > 0$ is subharmonic as $Vf_0 > \tilde{V}\tilde{f}_0$. Hence, its maximum occurs on the boundary, but we have $g = 0$ there. This contradicts $g(|x|) > 0$ on $\Omega$.
5. Equation (2.5.6) is obtained by using equation (2.5.4) and Stokes:

$$\mathcal{E}_R(\phi_0) = \int_{B_R}\Big(\nabla\phi_0(r)^2 + \frac{1}{2}V\phi_0^2\Big)dx = \int_{B_R}\nabla\Big(\phi_0\nabla\phi_0\Big)dx = 4\pi a[(1-aR^{-1})]^{-1}. \tag{2.5.8}$$

□

To prepare us for the rigorous mathematical use of the scattering equation we have to ensure that the scattering process happens in a ball that fits into our box $[-L/2, L/2]^3$. To guarantee this, we consider the scattering process to happen on a ball of radius $\ell \leq L/2$ and continue the solution outside of $B_\ell$ with the constant function 1. Furthermore, we enforce Neumann boundary condition $\frac{\partial\phi}{\partial n} = 0$ where $n$ denotes the boundary normal. However, this has the disadvantage that (2.5.1) is not fullfilled anymore. Lemma 2.5.1 quantifies the effect of the cutoff with the Neumann boundary condition.
In the rest of this section we closely follow [2]. As we will later rescale variables we define the lowest energy solution $f_\ell$ of the Neumann problem

$$\Big[-\Delta + \frac{1}{2}V\Big]f_\ell = \lambda_\ell f_\ell \tag{2.5.9}$$

on the ball $|x| \leq N^{1-\kappa}\ell$ with $0 < \ell < 1/2$ and $0 \leq \kappa \leq 1$. We normalize $f_\ell(x) = 1$ if $|x| = N^{1-\kappa}\ell$ and by rescaling define $f_N := f_\ell(N^{1-\kappa}x)$ for $|x| \leq \ell$. For $x \in \Lambda = [-1/2, 1/2]^3$ the rescaled Neumann problem then reads as follows

$$\Big[-\Delta + \frac{1}{2}N^{2-2\kappa}V(N^{1-\kappa}x)\Big]f_N(x) = N^{2-2\kappa}\lambda_\ell f_N(x)\chi_\ell(x). \tag{2.5.10}$$

The proof of our main result relies heavily on the second quantization formalism in the Fourier basis. Therefore we need a Fourier transformed version of the Neumann problem. The Fourier coefficients

[12] See Theorem 9.4 in [16]

of $w_N(x) := 1 - f_N(x)$ are given by

$$\hat{w}_N(p) = \int_\Lambda w_\ell(N^{1-\kappa}x)e^{-ip\cdot x}dx = \frac{1}{N^{3-3\kappa}}\hat{w}_\ell(p/N^{1-\kappa}) \tag{2.5.11}$$

where $w_\ell(x) := 1 - f_\ell(x)$ and $p \in \Lambda^*$ with $\Lambda^* := 2\pi/L\mathbb{Z}^3$. Furthermore, for the construction of the trial state the coefficients $\eta : \Lambda^* \mapsto \mathbb{R}$ with

$$\eta(p) = -N\hat{w}_N(p) = -\frac{N^\kappa}{N^{2-2\kappa}}\hat{w}_\ell(p/N^{1-\kappa}) \tag{2.5.12}$$

will be of importance. For convenience we denote them by $\eta_p$. The Neumann problem written in terms of these coefficients looks as follows:

$$p^2\eta_p + \frac{N^\kappa}{2}\hat{V}(p/N^{1-\kappa}) + \frac{1}{2N}\sum_{q\in\Lambda^*} N^\kappa\hat{V}((p-q)/N^{1-\kappa})\eta_q = N^{3-2\kappa}\lambda_\ell(\hat{\chi}_\ell * \hat{f}_N)(p). \tag{2.5.13}$$

The above equation can be derived by Fourier transforming equation (2.5.10), applying the convolution theorem and then rewriting $\hat{f}_N(p)$ with $\eta_p$.
The following Lemma from [2] summarizes some important properties of the eigenvalue problem (2.5.9). The proof can be found in [4, Appendix A] with the replacement $N \in \mathbb{N}$ by $N^{1-\kappa}$.

**Lemma 2.5.1.** *Let $V \in L^3(\mathbb{R}^3)$ be nonnegative, compactly supported and spherically symmetric. Fix $\ell > 0$ and let $f_\ell$ denote the solution of* (2.5.9)*. For $N \in \mathbb{N}$ large enough the following properties hold true.*

1. *We have*
$$\left|\lambda_\ell - \frac{3a}{N^{3-3\kappa}\ell^3}\right| \leq \frac{1}{N^{3-3\kappa}\ell^3}\frac{Ca^2}{N^{1-\kappa}\ell}. \tag{2.5.14}$$

2. *We have $0 \leq f_\ell$, $w_\ell \leq 1$. Moreover there exists a constant $C > 0$ such that*
$$\left|\int V(x)f_\ell(x)dx - 8\pi a\right| \leq \frac{Ca^2}{N^{1-\kappa}\ell}. \tag{2.5.15}$$

3. *There exists a constant $C > 0$ such that, for all $x \in \mathbb{R}^3$,*
$$w_\ell(x) \leq \frac{C}{1+|x|} \quad \textit{and} \quad |\nabla w_\ell(X)| \leq \frac{C}{1+x^2}. \tag{2.5.16}$$

4. *There exists a constant $C > 0$ such that, for all $p \in \mathbb{R}^3 \setminus \{0\}$,*
$$|\hat{w}_N(p)| \leq \frac{C}{N^{1-\kappa}p^2}. \tag{2.5.17}$$

   *In particular we have for all $p \in \Lambda_+^*$*
$$|\eta_p| \leq \frac{CN^\kappa}{p^2} \quad \textit{and} \quad |\eta_0| \leq CN^\kappa. \tag{2.5.18}$$

# 3 Main Result

We prove an upper bound for the free energy of a Bose gas at positive temperature on the torus $\Lambda_L := \mathbb{R}^3/L\mathbb{Z}^3$ in the Gross-Pitaevskii limit. As already mentioned in the introduction, in the Gross-Pitaevskii regime we consider interactions in the same order of magnitude as the spectral gap of the Laplacian. Moreover, we take a combined limit $N \to \infty$ and $\varrho^{2/3}\beta \sim 1$ where $N$ is the particle number, $\beta$ the inverse temperature and $\varrho$ the density.
The system is investigated in a grand canonical setting. This means the particle number $N$ is not fixed and the states are defined as operators acting on the bosonic Fock space $\mathscr{F}(L^2(\Lambda_L))$. To be able to take a plausible limit $N \to \infty$ we investigate the system for states with particle expectation $N$ as it is done in [8]. Specifically, for states in the following set

$$\mathscr{S}_N^{\mathrm{gc}} := \Big\{\Gamma \in \mathcal{B}(\mathscr{F}(L^2(\Lambda_L)))\Big|\Gamma \geq 0, \mathrm{Tr}\,[\Gamma] = 1, \mathrm{Tr}\,[\mathcal{N}\Gamma] = N, \mathrm{Tr}\,[H_N\Gamma] < \infty\Big\}, \tag{3.0.1}$$

where $H_N$ is the Hamiltonian of the system and $\mathcal{N}$ the particle number operator. For convenience we work from now on with the inverse temperature $\beta$ instead of the temperature $T$. The Gibbs free energy functional for states in $\mathscr{S}_N$ is defined analogously to (2.3.4):

$$\mathcal{F}(\Gamma) := \mathrm{Tr}\,[H_N\Gamma] - \frac{1}{\beta}S(\Gamma). \tag{3.0.2}$$

The grand canonical version of the free energy is then defined as

$$F(N, \Lambda_L, \beta) := \inf_{\Gamma \in \mathscr{S}_N^{\mathrm{gc}}} \mathcal{F}(\Gamma) = -\frac{1}{\beta}\ln\Big(\mathrm{Tr}\Big[\exp\big(-\beta(H_N - \mu\mathcal{N})\big)\Big]\Big) + \mu N. \tag{3.0.3}$$

Here the chemical potential $\mu$ is chosen such that for the Gibbs state

$$\Gamma_{\mathrm{G}} := \frac{\exp(-\beta(H_N - \mu\mathcal{N}))}{\mathrm{Tr}\,[\exp(-\beta(H_N - \mu\mathcal{N}))]} \tag{3.0.4}$$

$\mathrm{Tr}\,[\mathcal{N}\Gamma_{\mathrm{G}}] = N$ holds. Note that the Gibbs state (3.0.4) is the unique minimizer of the Gibbs free energy functional (3.0.2).
To have the interaction of the same order of magnitude as the spectral gap of the Laplacian we consider potentials with scattering length $a_N \sim L/N$. Thus for $n$ particles the Hamiltonian of the system takes the form

$$H_N^{(n)} = \sum_{i=1}^{n} -\Delta_i + \sum_{1\leq i<j\leq n} \big(N/L\big)^2 V\Big(N/Ld(x_i, x_j)\Big), \tag{3.0.5}$$

where $V \in L^3(\mathbb{R}^3)$ is chosen to be nonnegative, radial and compactly supported with scattering length $a$. $\Delta_i$ denotes the Laplacian with periodic boundary conditions acting on the $i$-th factor of the tensor product. The distance between two points $x, y \in \Lambda_L$ is defined by $d(x, y) := \min_{k\in\mathbb{Z}^3} |x - y - kL|$.

**Theorem 3.0.1.** *Assume that $V \in L^3(\mathbb{R}^3)$ is nonnegative, radial and compactly supported with a fixed scattering length $a > 0$. Assume that $\beta \geq \beta_c(1+\delta)$ where $\delta > 0$ and $\beta_c$ is the inverse critical temperature of the ideal Bose gas. Denote by $\mu_0$ and $\varrho_0(N, \Lambda_L, \beta)$ the chemical potential and the expected condensate density of the ideal Bose gas with particle expectation N, respectively. In the combined limit $N \to \infty$ with $\varrho^{2/3}\beta$ fixed and $a_N = aL/N$, for any $0 < \varepsilon < 1/6$ we have*

$$F(N, \Lambda_L, \beta) \leq F_0^{\text{th}}(N_{\text{th}}, \Lambda_L, \beta) + 4\pi a_N |\Lambda_L| \Big(2\varrho^2 - \varrho_0^2(N, \Lambda_L, \beta)\Big) + \frac{1}{2\beta} \ln\Big(\beta 4 a_N |\Lambda_L|^{-1}\Big) + O\Big(L^{-2} N^{1/2+\varepsilon}\Big). \tag{3.0.6}$$

*Here $F_0^{\text{th}}(N_{\text{th}}, \Lambda_L, \beta)$ denotes the free energy of the thermal cloud of the ideal Bose gas given by*

$$F_0^{\text{th}}(N_{\text{th}}, \Lambda_L, \beta) = \frac{1}{\beta} \sum_{p \in (2\pi/L)\mathbb{Z}^3 \setminus \{0\}} \ln\Big(1 - \exp\big(-\beta(p^2 - \mu_0)\big)\Big) + \mu_0 N_{\text{th}}, \tag{3.0.7}$$

*where $N_{\text{th}} = N - |\Lambda_L| \varrho_0(N, \Lambda_L, \beta)$.*

**Remarks 3.0.1.**

1. Notice the scaling of the terms: $F_0^{\text{th}}(N_{\text{th}}, \Lambda_L, \beta) \sim L^{-2} N^{5/3}$, $4\pi a_N |\Lambda_L| \big(2\varrho^2 - \varrho_0^2(N, \Lambda_L, \beta)\big) \sim L^{-2} N$ and $(2\beta)^{-1} \ln(\beta 4 a_N |\Lambda_L|^{-1}) \sim L^{-2} N^{2/3} \ln(N)$.

2. The error for the upper bound of the canonical free energy obtained in [9] turned out to be $O(L^{-2}N^{2/3})$. Assuming a grand canonical setting we are able to improve the error to $O(L^{-2}N^{1/2+\varepsilon})$ for any $0 < \varepsilon < 1/6$.

3. It was shown in [22] and [30] that the second order correction also holds in the thermodynamic limit. According to [9] this is consistent because we can interpret our limit as a combined thermodynamic and dilute limit.

4. For $\beta \leq \beta_c$ the leading order in the interaction energy is given by $8\pi a_N |\Lambda_L| \varrho^2$. This should be compared to $4\pi a_N |\Lambda_L| \varrho^2$, which is the interaction energy at zero temperature. As remarked in [9], this additional factor of two arises from an exchange effect with its origin in the symmetrization of the wave-function. This effect is only noticeable if the particles occupy different states. As particles in the condensate occupy the same state, this effect only becomes visible if the system has nonzero temperature. This in particular explains the factor $2\varrho^2 - \varrho_0^2(N, \Lambda_L, \beta)$ in the second order term.

5. The assumption $\beta \geq \beta_c(1+\delta)$, where $\delta > 0$, ensures with equation (2.4.12) that there is a sufficient amount of particles in the condensate. For $\beta < \beta_c(1+\delta)$ the bound (3.0.6) can be derived without the third order term. Thus also recovering the same second order correction as obtained in [9] for a canonical setting.

6. Note that, instead of the canonical free energy of the ideal Bose gas as derived in [9], we only obtained the grand canonical free energy of the thermal cloud of the ideal Bose gas. This is because the entropy of the condensate is absorbed into the third order correction.

7. In the combined limit we have $\beta 4 a_N |\Lambda_L|^{-1} \sim N^{-5/3}$. Thus the third term on the r.h.s of (3.0.6) actually lowers the upper bound. This correction arises due to an increase in the entropy of the condensate. Although, this rise is connected with an increase in interaction energy of the

condensate, the entropy contribution predominates and therefore lowers the upper bound. Also note that the contribution of the third term in (3.0.6) to the energy per unit volume would vanish in the thermodynamic limit.

8. The next order term is expected to be of the order of magnitude $L^{-2}N^{2/3}$ and lowers the free energy. This in particular implies that for a lower bound we would not be able to obtain an error smaller than $O(L^{-2}N^{2/3})$ without considering this fourth order correction. To derive it we would need to write the Hamiltonian as a sum of an operator acting only on the non-condensed particles and the Bogoliubov Hamiltonian $H_{\mathrm{B}}$. The operator $H_{\mathrm{B}}$ can be diagonalized by an appropriate Bogoliubov transformation. We therefore expect that $F_0^{\mathrm{th}}(N_{\mathrm{th}}, \Lambda_L, \beta)$ needs to be replaced by the free energy of an ideal Bose gas with dispersion relation

$$\varepsilon(p) = \sqrt{(p^2 - \mu)^2 + 16\pi a_N \varrho_0(N, \Lambda_L, \beta)(p^2 - \mu)}. \tag{3.0.8}$$

Then the difference of the free energies is in the order of $L^{-2}N^{2/3}$.

# 4 Proof of the Main Theorem

In this chapter we prove Theorem 3.0.1. To guide the reader we describe first the main steps of the proof in the following subsection.

## 4.1 Proof Strategy

The proof strategy is similar to the strategy used to prove the upper bound in [9]. However, in this proof we work in a grand canonical instead of a canonical setting. Additionally, we derive a third order contribution arising from the entropy and the interaction energy of the condensate.
The main idea of the proof is based on the characterization of the free energy by the Gibbs variational principle (3.0.3). To exploit it, we construct a trial state such that its free energy can be bounded from above by the r.h.s of (3.0.6).
As a starting point we choose the Gibbs state of the ideal Bose gas (3.0.4). On the basis of this we will extract the free energy of the thermal cloud of the ideal Bose gas.
To obtain the interaction energy we add a correlation structure. The correlation structure is chosen such that it decreases the probability of finding two particles close together according to the solution of the scattering equation. This has the advantages that we can apply the scattering equation and naturally obtain the scattering length (see the bound (2.5.15)).
In order to make the computations less tedious, we add momentum cutoffs to the Gibbs state and the correlation structure. Based on this, we work mainly in the Fourier basis and write the operators in their second quantized form according to this basis. This has the advantage that the one-particle density matrix of the ideal Bose gas is diagonal with the specific expression given in equations (2.4.4) and (2.4.5). Furthermore, the momentum cutoffs can be naturally defined in this basis.
The new contribution to the free energy is obtained by exchanging the condensate of the ideal Bose gas with a certain linear combination of coherent condensate states.

## 4.2 Construction of the Trial State

For convenience we rescale variables $x_j \to x_j/L$. As someone might want to extend this proof to the thermodynamic limit, we also include the paramater $\kappa$ corresponding to the parameter $\kappa$ introduced in [2]. There, a diagonal limit with $L = \tilde{\varrho}^{-\gamma}$ for $\gamma > 1$ is considered. Furthermore, they set $N = \tilde{\varrho}^{1-3\gamma}$ and defined $\kappa := (2\gamma - 1)/(3\gamma - 1)$ which implies $\kappa \in (1/2, 2/3)$. In the end they optimized over $\gamma$. As we will not need this Ansatz we simply think of $\kappa$ being 0. The rescaling implies that (3.0.5) is unitarily equivalent to $L^{-2}H_N$, where $H_N$ acts on the bosonic Fock space $\mathscr{F}(L^2(\Lambda))$ with $\Lambda := \mathbb{R}^3/\mathbb{Z}^3$.

On the subspace of $\mathscr{F}(L^2(\Lambda))$ restricting to $n$-particle wave-functions we have $(H_N\psi)^{(n)} = H_N^{(n)}\psi$ with

$$H_N^{(n)} = \sum_{i=1}^{n} -\Delta_i + \sum_{1\le i<j\le n} N^{2-2\kappa} V\Big(N^{1-\kappa} d(x_i, x_j)\Big). \tag{4.2.1}$$

Let $\{u_p\}_{p\in\Lambda^*}$ be the Fourier basis of $L^2(\Lambda)$ with $u_p(x) = \exp(-ipx)$ and $\Lambda^* = 2\pi\mathbb{Z}^3$. Define by $a_p^* := a_+^*(u_p)$, $a_p := a_+(u_p)$ the corresponding bosonic creation and annihilation operators with the canonical commutation relations

$$[a_p, a_q] = [a_p^*, a_q^*] = 0, \qquad [a_p, a_q^*] = \delta_{p,q}. \tag{4.2.2}$$

As dervied in (2.1.20), we can express the Hamiltonian (4.2.1) in terms of bosonic creation and annihilation operators

$$H_N = \sum_{p\in\Lambda^*} p^2 a_p^* a_p + \frac{1}{2N^{1-\kappa}} \sum_{p,u,v\in\Lambda^*} \hat{V}(p/N^{1-\kappa}) a_{u+p}^* a_{v-p}^* a_u a_v =: H_0 + \mathcal{V}_N. \tag{4.2.3}$$

Let us start with the construction of the trial state. Consider the Gibbs state $\Gamma_G$ of the ideal Bose gas with the chemical potential $\mu_0$ chosen such that $\mathrm{Tr}[\mathcal{N}\Gamma_G] = N$. Note that this implies $\mu_0 < 0$.
The first modification is to exchange the condensate of $\Gamma_G$ with a coherent condensate. This will later lower the interaction energy from $8\pi a_N|\Lambda_L|\varrho^2$ to $4\pi a_N|\Lambda_L|\Big(2\varrho^2 - \varrho_0^2(N,\Lambda_L,\beta)\Big)$ where $\varrho_0(N,\Lambda_L,\beta)$ is the condensate density.
Due to Lemma 2.1.1 we can identify $\mathscr{F}(L_0^2(\Lambda)\oplus L_>^2(\Lambda))$ with $\mathscr{F}_0\otimes\mathscr{F}_> := \mathscr{F}(L_0^2(\Lambda))\otimes\mathscr{F}(L_>^2(\Lambda))$ where $L_0^2(\Lambda)$ is the linear space spanned by the constant function and $L_>^2(\Lambda)$ its orthogonal complement. Thus, we can split the Fock space into wave-functions of condensed particles and wave-functions of the thermal cloud.
On the condensate Fock space $\mathscr{F}_0$ we consider coherent wave-functions of the form (2.2.11). As the states $|z\rangle\langle z|$ for $z\in\mathbb{C}$ are one-dimensional projections, they have zero entropy. In order to gain some entropy contribution we define the following probability distribution

$$f(x) = \frac{\exp\Big(-\Big(\lambda_1 N_0^{-1} x + \lambda_2 N_0^{-2} x^2\Big)\Big)}{N_0 Z(\lambda_1,\lambda_2)} \quad \text{where} \tag{4.2.4}$$
$$Z(\lambda_1,\lambda_2) = \int_0^\infty \exp\Big(-\Big(\lambda_1 x + \lambda_2 x^2\Big)\Big)dx.$$

The procedure to incorporate this distribution into the condensate is the same as described in [8]. The pair $(\lambda_1,\lambda_2)$ is chosen such that we have

$$\int_0^\infty x f(x)dx = \frac{N_0}{Z(\lambda_1,\lambda_2)} \int_0^\infty x\exp\Big(-(\lambda_1 x + \lambda_2 x^2)\Big)dx = N_0, \tag{4.2.5}$$
$$\int_0^\infty x^2 f(x)dx = \frac{N_0^2}{Z(\lambda_1,\lambda_2)} \int_0^\infty x^2\exp\Big(-\Big(\lambda_1 x + \lambda_2 x^2\Big)\Big)dx = N_0^2(1+g(N_0)), \tag{4.2.6}$$

where $0 < g(N_0) \ll 1$. In the next section the existence of a pair $(\lambda_1,\lambda_2)$ complying with (4.2.5) as well as (4.2.6) is proven. We will see that the condition $0 < g(N_0) \ll 1$ can only be fulfilled if we assume $\beta \ge \beta_c(1+\delta)$ where $\delta > 0$. It should also be noted that we choose the exact value of $N_0$ later

in the proof. Moreover, the slightly higher second moment, defined in (4.2.6), gives us a parameter $g(N_0)$ to optimize over. The probability distribution of the form (4.2.4) minimizes the entropy with the constraints (4.2.5) and (4.2.6) for the first and second moments. This can be shown by variational methods but is omitted here.
The ideal gas state with exchanged condensate is defined as

$$\Gamma_0 := \left( \int_{\mathbb{C}} f(|z|^2) \, |z\rangle \langle z| \, dz \right) \otimes \Gamma^0_{\mu_0}, \tag{4.2.7}$$

where

$$\Gamma^0_{\mu_0} := \frac{\exp\left(-\beta d\Gamma\left(-\Delta - \mu_0\right)\right) \chi(\mathcal{N}_0 = 0)}{\mathrm{Tr}_{\mathscr{F}_>}\left[\exp\left(-\beta d\Gamma\left(-\Delta - \mu_0\right)\right) \chi(\mathcal{N}_0 = 0)\right]}, \tag{4.2.8}$$

with $\mathcal{N}_0 := a_0^* a_0$ and $dz$ is the measure defined in (2.2.13). By $\chi(\mathcal{N}_0 = 0)$ we denote the operator corresponding to the indicator function $\chi(\{0\})$ (corresponding in the sense of functional calculus applied to $\mathcal{N}_0$).
Let $g : [0, \infty) \to \mathbb{R}$ s.t. $g \in L^1([0, \infty))$. Notice that we have

$$\int_{\mathbb{C}} g(|z|^2) dz = 2 \int_0^\infty g(r^2) r dr = \int_0^\infty g(x) dx \tag{4.2.9}$$

where we transformed into polar coordinates in the first equality and in the second equality we performed the change of variable $r \mapsto \sqrt{x}$.
For computational reasons, we would like our modified ideal gas state to only contain momenta with $|p| \leq N^{1/3+\delta_L}$ for some $\delta_L > 0$. Thus we define the following sets

$$P_L := \left\{ p \in \Lambda^* : |p| \leq N^{1/3+\delta_L} \right\}, \tag{4.2.10}$$

$$P_H := \left\{ p \in \Lambda^* : |p| \geq N^{1-\delta_H} \right\}. \tag{4.2.11}$$

Here $\delta_L, \delta_H > 0$ such that $\delta_L + \delta_H < 2/3$. In the following we denote $\mathcal{N}_{P_L^c,0} := a_0^* a_0 + \sum_{p \in P_L^c} a_p^* a_p$.
Incorporating the cutoff, our trial state then looks as follows

$$\tilde{\Gamma}_0 := \left( \int_{\mathbb{C}} f(|z|^2) \, |z\rangle \langle z| \, dz \right) \otimes \Gamma^{\mathrm{ec}}_{\mu} = \sum_{\alpha=1}^{\infty} \lambda_\alpha \, |\psi_\alpha\rangle \langle \psi_\alpha| \, , \tag{4.2.12}$$

where

$$\Gamma^{\mathrm{ec}}_{\mu} := \frac{\exp\left(-\beta d\Gamma\left(-\Delta - \mu\right)\right) \chi(\mathcal{N}_{P_L^c,0} = 0)}{\mathrm{Tr}_{\mathscr{F}_>}\left[\exp(-\beta d\Gamma(-\Delta - \mu)) \chi(\mathcal{N}_{P_L^c,0} = 0)\right]}. \tag{4.2.13}$$

In (4.2.12) we expanded in an orthonormal subset $\{\psi_\alpha\}_{\alpha=1}^\infty$ of $\mathscr{F}_0 \otimes \mathscr{F}_>$ such that for $\psi_\alpha = f \otimes g$ with $f \in \mathscr{F}_0$ and $g \in \mathscr{F}_>$ we have that $g$ is a symmetric tensor product of plane waves with non-zero momenta.
Notice that the chemical potential $\mu$ for the thermal state with the cutoff is different from $\mu_0$. This comes from the fact that we want to keep the particle number expectation fixed. Therefore $\mu$ and $\mu_0$ are defined as

$$\mathrm{Tr}_{\mathscr{F}_>}\left[\mathcal{N}\Gamma^0_{\mu_0}\right] = \mathrm{Tr}_{\mathscr{F}_>}\left[\mathcal{N}\Gamma^{\mathrm{ec}}_{\mu}\right] = N_{\mathrm{th}} \quad \text{where} \quad N_{\mathrm{th}} := N - \tilde{N}_0. \tag{4.2.14}$$

Here $\tilde{N}_0$ denotes the expected number of particles in the condensate of the ideal Bose gas. In order for the above equation to be well-defined we need to have $\mu < 4\pi^2$.
Let us show that (4.2.12) indeed defines a state. It is clear that $\tilde{\Gamma}_0 \geq 0$. Thus, we can assume without loss of generality $\lambda_\alpha > 0$ for all $1 \leq \alpha < \infty$. To show that $\mathrm{Tr}\,[\tilde{\Gamma}_0] = 1$, we use the fact that $\mathrm{Tr}_{\mathscr{F}_0 \otimes \mathscr{F}_>}[A \otimes B] = \mathrm{Tr}_{\mathscr{F}_0}[A]\,\mathrm{Tr}_{\mathscr{F}_>}[B]$ where $A, B$ are trace class operators on $\mathcal{F}_0$ and $\mathscr{F}_>$, respectively. Also applying linearity of the trace and equation (4.2.9) we compute

$$\mathrm{Tr}_{\mathscr{F}_0 \otimes \mathscr{F}_>}[\tilde{\Gamma}_0] = \left( \int_{\mathbb{C}} f(|z|^2)\,\mathrm{Tr}\left[\, |z\rangle\langle z| \,\right] dz \right) \mathrm{Tr}_{\mathscr{F}_>}[\Gamma_\mu^{\mathrm{ec}}] = \int_{\mathbb{C}} f(|z|^2) dz = \int_0^\infty f(x) dx = 1$$

Note that the above implies $\sum_{\alpha=1}^\infty \lambda_\alpha = 1$. To simplify the notation we will from now on omit to denote over which space we take the trace.

We will use the following operator to add correlation to our modified ideal gas state:

$$\eta := \frac{1}{2N} \sum_{p \in P_H, u, v \in P_L} \eta_p a_{u+p}^* a_{v-p}^* a_u a_v. \tag{4.2.15}$$

Remember that $\eta_p = -N\hat{w}_N(p)$ and $w_N(x) = 1 - f_N(x)$ where $f_N$ is the solution of equation (2.5.10). Lemma 2.5.1 tells us that $0 \leq f_N(x) \leq 1$ for $x < \ell$. Furthermore, we have $f_N(x) = 1$ for $x \geq \ell$. Thus we see that $\eta_p$ is the Fourier transform of a function that is negative on an interparticle distance $x < \ell$ and 0 for $x \geq \ell$. Thus the operator $1 + \eta$ lowers the probability of two particles being close together according to the scattering equation. Finally, we choose the trial state to be

$$\Gamma := \sum_{\alpha=1}^\infty \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha| \quad \text{where} \quad \phi_\alpha := \frac{(1+\eta)\psi_\alpha}{\|(1+\eta)\psi_\alpha\|}. \tag{4.2.16}$$

As $\Gamma$ is a linear combination of one-dimensional projections with positive coefficients we certainly have $\Gamma \geq 0$. Note also

$$\mathrm{Tr}\,[\Gamma] = \sum_{\alpha=1}^\infty \lambda_\alpha\,\mathrm{Tr}\left[\, |\phi_\alpha\rangle\langle\phi_\alpha| \,\right] = \sum_{\alpha=1}^\infty \lambda_\alpha = 1.$$

It remains to show that $\mathrm{Tr}[\mathcal{N}\Gamma] = N$. In section 4.4 we prove the estimate

$$\mathrm{Tr}[\mathcal{N}\Gamma] = N_0 + N_{\mathrm{th}} + O\Big(N^{\delta_H + 2\kappa}\Big). \tag{4.2.17}$$

Therefore we choose $N_0$ such that we have $\mathrm{Tr}[\mathcal{N}\Gamma] = N$. This, together with the estimate (4.2.17) implies

$$|N_0 - \tilde{N}_0| \leq C N^{\delta_H + 2\kappa}. \tag{4.2.18}$$

Remember that $\tilde{N}_0 = N - N_{\mathrm{th}}$ is the expected number of particles in the condensate of the ideal Bose gas with chemical potential $\mu_0$.

## 4.3 Preparatory Lemmas

In all proofs and estimations we denote by $C > 0$ an arbitrary constant independent of $N$, whose precise value may change from line to line.
To give integral estimates to sums over momenta we need the following technical Lemma which can be found in [9, Lemma 3.3.].

**Lemma 4.3.1.** *Let $f : [0, \infty) \to \mathbb{R}$ be a nonnegative and monotone decreasing function and choose some $\lambda \geq 0$. Then*

$$\sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} f(|p|)\chi(|p| \geq \lambda) \leq \frac{1}{(2\pi)^3} \int_{|p| \geq [\lambda - \sqrt{12}\pi]_+} f(|p|)\left(1 + \frac{3\pi}{|p|} + \frac{6\pi}{p^2}\right) dp \tag{4.3.1}$$

*holds.*

*Proof.* Assume first that $\lambda - \sqrt{12}\pi \leq 0$. In this case we drop the characteristic function on the left-hand side of (4.3.1) for an upper bound. Next, we write the sum over $p$ as the sum over those $p$ that are an element of one of the coordinate planes, i.e. with one coordinate $p_i$ equal to zero, plus a sum over all remaining $p$. To estimate the sum over all remaining $p$, we interpret the sum as a lower Riemann sum and find that it is bounded from above by

$$\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} f(|p|)dp. \tag{4.3.2}$$

The sum over those $p$ that are an element of the coordinate planes can be estimated similarly. Here we write the whole sum as a sum over those $p$ that are an element of one of the coordinate axes plus the sum over all remaining $p$. The sum over the remaining $p$ is estimated again by interpreting it as a lower Riemann sum. For one such coordinate plane, we find

$$\sum_{p \in 2\pi\mathbb{Z}^2 \cap \{p_i \neq 0 \text{ for } i=1,2\}} f(|p|) \leq \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} f(|p|)dp. \tag{4.3.3}$$

Because there are three coordinate planes, we have three such terms. It remains to estimate the sum over those $p$ that are an element of one of the coordinate axes of $\mathbb{R}^3$. Again by interpreting the sums over the three coordinate axis as lower Riemann sums, we find that they are bounded from above by

$$\frac{3}{\pi} \int_0^\infty f(|p|)dp. \tag{4.3.4}$$

In order to write the two-dimensional integral from (4.3.3) in terms of a three-dimensional integral, we use

$$\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} f(|p|)dp = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} f(|p|)\frac{\pi}{|p|}dp. \tag{4.3.5}$$

A similar computation can be done for the term in Equation (4.3.4). Putting these estimates together proves (4.3.1) in this case. The bound in the case $\lambda - \sqrt{12}\pi \geq 0$ can be obtained similarly. Here we only have to realize that $\lambda - \sqrt{12}\pi$ is the radius of the largest ball such that the integral over its complement is an upper bound to the relevant three-dimensional lower Riemann sum. This proves the claim. □

Using this Lemma we can estimate for $\lambda \geq 1 + \sqrt{12}\pi$ and $f : [0, \infty) \to \mathbb{R}$ a positive, monotone decreasing and radially symmetric function with $f(|\cdot|) \in L^1(\mathbb{R}^3)$

$$\sum_{p \in \Lambda_+^*} f(|p|)\chi(|p| \geq \lambda) \leq C \int_{|p| \geq \lambda - \sqrt{12}\pi} f(|p|)dp = C \int_{\lambda - \sqrt{12}\pi}^{\infty} f(|p|)p^2 dp. \tag{4.3.6}$$

From now on we will not explicitally reference Lemma 4.3.1 and just apply the bound (4.3.6) if the conditions for this estimate are fullfilled. The following Lemma is a simple application of the bound (4.3.6).

**Lemma 4.3.2.** *There exists a constant $C > 0$ such that for $N$ large enough we have*

$$\|\eta\|^2_{L^2(P_H)} \leq CN^{-1+\delta_H+2\kappa}. \tag{4.3.7}$$

*Proof.* We use (2.5.18) and (4.3.6) to show that

$$\|\eta\|^2_{L^2(P_H)} = \sum_{p \in P_H} |n_p|^2 \leq CN^{2\kappa} \int_{N^{1-\delta_H} - \sqrt{12}\pi}^{\infty} \frac{1}{p^2} dp \leq CN^{2\kappa} \left(N^{1-\delta_H} - \sqrt{12}\pi\right)^{-1} \leq CN^{\delta_H - 1 + 2\kappa}$$

holds. □

We will frequently use the fact that the probability of finding particles with momenta higher than $N^{1/3}$ in the Gibbs state $\Gamma_0$ is exponentially small. This is made precise by the following Lemma. Recall that $\delta_L + \delta_H < 2/3$, $\delta_H > 0, \delta_L > 0$.

**Lemma 4.3.3.** *Assume $\mu < 4\pi^2$. There exists $C > 0$ such that for $N$ large enough we have*

$$\sum_{p \in P_L^c} \hat{\gamma}_0(p) \leq O\left(\exp\left(-CN^{2\delta_L}\right)\right).$$

*Proof.* Using the expression (2.4.5) for the Fourier transform of the one-particle density matrix, the assumption $\mu < 4\pi^2$ and the bound (4.3.6) we can estimate for $N$ large

$$\begin{aligned} \sum_{p \in P_L^c} \hat{\gamma}_0(p) &= \sum_{p \in P_L^c} \frac{1}{\exp\left(\beta\left(p^2 - \mu\right)\right) - 1} \\ &\leq C \sum_{p \in P_L^c} \exp\left(-\beta p^2\right) \leq C \int_{N^{1/3+\delta_L} - \sqrt{12}\pi}^{\infty} p^2 \exp\left(-\beta p^2\right) dp. \end{aligned} \tag{4.3.8}$$

Recall that we can write $\beta = \beta_0 N^{-2/3}$ where $\beta_0$ is a positive constant independent of $N$. Let $c > 0$, then we find for any $r \in \mathbb{R}$ and $N$ large enough a constant $C_r > 0$ independent of $N$ such that

$$\sup_{N^{1/3+\delta_L} - \sqrt{12}\pi \leq p < \infty} p^r \exp\left(-c\beta p^2\right) < C_r. \tag{4.3.9}$$

Using this bound we estimate for the r.h.s of (4.3.8)

$$\begin{aligned}\int_{N^{1/3+\delta_L}-\sqrt{12}\pi}^{\infty} \exp\left(-\beta p^2\right) p^2 dp &\leq \sup_{N^{1/3+\delta_L}-\sqrt{12}\pi \leq q<\infty} \left[q \exp\left(-\frac{\beta}{2}q^2\right)\right] \int_{N^{1/3+\delta_L}-\sqrt{12}\pi}^{\infty} \exp\left(-\frac{\beta}{2}p^2\right) p dp \\ &\leq CN^{2/3} \exp\left(-\frac{\beta}{2}\left(N^{1/3+\delta_L} - \sqrt{12}\pi\right)^2\right) \leq C \exp\left(-\frac{\beta_0}{4}\left(N^{\delta_L} - \sqrt{12}\pi N^{-1/3}\right)^2\right) \\ &\leq O\left(\exp\left(-CN^{2\delta_L}\right)\right), \end{aligned} \tag{4.3.10}$$

which proves the Lemma. □

The following result shows that the probability of having significantly more than $N_{\mathrm{th}}$ particles in the thermal Gibbs state with the momentum cutoff is exponentially small.

**Lemma 4.3.4.** *Assume $\mu < 0, c > 1$ and let $p \in \mathbb{N}_0$, then we have*

$$\mathrm{Tr}\left[\mathcal{N}^p \chi(\mathcal{N} > cN_{\mathrm{th}}) \Gamma_\mu^{\mathrm{ec}}\right] \leq O\left(\exp\left(-CN^{1/3-\varepsilon}\right)\right). \tag{4.3.11}$$

*Here $1/3 > \varepsilon > 0$ and $C > 0$.*

*Proof.* We first show the inequality for $p = 0$. Let $\beta\pi \geq k > 0$. Note that we have $d\Gamma(-\Delta) \geq 4\pi^2 \mathcal{N}_{P_L} > k\beta^{-1}\mathcal{N}_{P_L}$ on $\mathscr{F}_>$. Thus we can write

$$\begin{aligned}\mathrm{Tr}\left[\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right] &\leq \mathrm{Tr}\left[\exp\left(k(\mathcal{N} - cN_{\mathrm{th}})\right)\Gamma_\mu^{\mathrm{ec}}\right] \\ &= \exp\left(-kcN_{\mathrm{th}}\right) \mathrm{Tr}\left[\exp\left(-\beta d\Gamma\left(-\Delta - \mu - \frac{k}{\beta}\right)\right)\chi(\mathcal{N}_{P_L^c} = 0)\frac{1}{Z_\mu^{\mathrm{ec}}}\right] \\ &= \exp\left(-kcN_{\mathrm{th}}\right) \exp\left(\beta(\Phi_\mu^{\mathrm{ec}} - \Phi_{\tilde{\mu}}^{\mathrm{ec}})\right). \end{aligned} \tag{4.3.12}$$

In the first line we used the estimate $\mathcal{N} > cN_{\mathrm{th}} \implies 1 \leq \exp\left(k(\mathcal{N} - cN)\right)$. In the third line we used that $d\Gamma(-\Delta - \mu)$ and $\mathcal{N}$ commute. This can easily be shown using their second quantization representation. In the third line we defined $\tilde{\mu} := \mu + \frac{k}{\beta}$ and wrote the trace in terms of the grand potentials corresponding to $\mu$ resp. $\tilde{\mu}$. The difference of the grand potentials can be estimated by

$$\begin{aligned}\beta(\Phi_\mu^{\mathrm{ec}} - \Phi_{\tilde{\mu}}^{\mathrm{ec}}) &= \sum_{p \in P_L \setminus \{0\}} \left[\ln\left(1 - \exp\left(-\beta(p^2 - \mu)\right)\right) - \ln\left(1 - \exp\left(-\beta\left(p^2 - \left(\mu + \frac{k}{\beta}\right)\right)\right)\right)\right] \\ &\leq \sum_{p \in P_L \setminus \{0\}} \frac{k}{\exp\left(\beta\left(p^2 - \left(\mu + \frac{k}{\beta}\right)\right)\right) - 1} \\ &\leq \sum_{p \in P_L \setminus \{0\}} \frac{k}{\exp\left(\beta(p^2 - \mu)\right) - 1} + \sum_{p \in P_L \setminus \{0\}} \frac{\exp\left(\beta\left(p^2 - \left(\mu + \frac{k}{\beta}\right)\right)\right)}{\left(\exp\left(\beta\left(p^2 - \left(\mu + \frac{k}{\beta}\right)\right)\right) - 1\right)^2} k^2 \\ &\leq kN_{\mathrm{th}}\left(1 + C\frac{k}{\beta^2 N_{\mathrm{th}}}\right). \end{aligned} \tag{4.3.13}$$

In the first inequality we used that $f(x) := \ln\left(1 - \exp\left(-\beta(p^2 - x)\right)\right)$ is a monotone decreasing, concave function for $x < p^2$ which holds in this case because $\mu < 0$ and $\frac{k}{\beta} \leq \pi < p^2$ for $p \in P_L \setminus \{0\}$.

Thus we have $f(\mu) \leq f(\mu + k\beta^{-1}) - f'(\mu + k\beta^{-1})k\beta^{-1}$. In the second inequality we argue similarly, using that $g(x) := (\exp(\beta(p^2 - x)) - 1)^{-1}$ is a monotone increasing, convex function. In the third inequality we used that the second term can be bounded by $C\beta^{-2}k^2$. This inequality can be found in [9, Lemma 3.3].
We combine (4.3.12) and (4.3.13) with the choice $k = \beta\pi$ and find

$$\begin{aligned}\mathrm{Tr}\left[\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right] &\leq \exp(-kcN_{\mathrm{th}})\exp\left(kN_{\mathrm{th}}\left(1 + C\frac{k}{\beta^2 N_{\mathrm{th}}}\right)\right)\\ &= \exp\left(-\pi\beta N_{\mathrm{th}}\left(c - 1 - C\frac{1}{\beta N_{\mathrm{th}}}\right)\right)\\ &\leq \exp\left(-CN^{1/3}\right). \end{aligned} \tag{4.3.14}$$

To obtain this bound we needed the assumption $c > 1, \beta = \beta_0 N^{-2/3}$ and that $N$ is large enough such that $\left(c - 1 - C(\beta N_{\mathrm{th}})^{-1}\right) > 0$. This proves the case $p = 0$.
Let us prove the bound for $p \in \mathbb{N}_+$. Choose an orthonormal basis of eigenfunction of $\mathcal{N}$ denoted by $\{\xi_\alpha\}_{\alpha=1}^\infty$ with corresponding eigenvalues $\{N_\alpha\}_{\alpha=1}^\infty$. Furthermore, denote $\lambda_\alpha^{\mathrm{ec}} = \langle \xi_\alpha, \Gamma_\mu^{\mathrm{ec}}\xi_\alpha\rangle$. Then we have by the triangle inequality

$$\begin{aligned}\left(\mathrm{Tr}\left[\mathcal{N}^p\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right]\right)^{1/p} &= \left(\sum_{\alpha=1}^\infty \lambda_\alpha^{\mathrm{ec}} N_\alpha^p \chi(N_\alpha > cN_{\mathrm{th}})\right)^{1/p}\\ &\leq \left(\sum_{\alpha=1}^\infty \lambda_\alpha^{\mathrm{ec}}(N_\alpha - N_{\mathrm{th}})^p\chi(N_\alpha > cN_{\mathrm{th}})\right)^{1/p} + \left(\sum_{\alpha=1}^\infty \lambda_\alpha^{\mathrm{ec}} N_{\mathrm{th}}^p \chi(N_\alpha > cN_{\mathrm{th}})\right)^{1/p}\\ &= \left(\mathrm{Tr}\left[(\mathcal{N} - N_{\mathrm{th}})^p\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right]\right)^{1/p} + N_{\mathrm{th}}\left(\mathrm{Tr}\left[\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right]\right)^{1/p}. \end{aligned} \tag{4.3.15}$$

The first term on the r.h.s of (4.3.15) can be estimated using that $\frac{k^p}{p!}(x - cN_{\mathrm{th}})^p \leq \exp(k(x - cN_{\mathrm{th}}))$ holds for $x > N_{\mathrm{th}}$ and then applying the same procedure as for the case $p = 0$:

$$\begin{aligned}\mathrm{Tr}\left[(\mathcal{N} - N_{\mathrm{th}})^p\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right] &= p!k^{-p}\,\mathrm{Tr}\left[\frac{k^p}{p!}(\mathcal{N} - N_{\mathrm{th}})^p\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right]\\ &\leq p!k^{-p}\,\mathrm{Tr}\left[\exp(k(\mathcal{N} - cN_{\mathrm{th}}))\Gamma_\mu^{\mathrm{ec}}\right]\\ &\leq p!k^{-p}\exp\left(-CN^{1/3}\right).\end{aligned}$$

We combine this bound, the estimate (4.3.14) and $N_{\mathrm{th}} \leq cN$ and find

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{N}^p\chi(\mathcal{N} > cN_{\mathrm{th}})\Gamma_\mu^{\mathrm{ec}}\right] &\leq \left(\left(N + (p!)^{1/p}k^{-1}\right)\exp(-CN^{1/3})\right)^p\\ &\leq CN^p\exp\left(-CN^{1/3}\right)\\ &\leq C_p\exp\left(-CN^{1/3-\varepsilon}\right)\end{aligned}$$

for some $1/3 > \varepsilon > 0$. □

In the following Lemma we quantify the difference in chemical potentials defined in (4.2.14). For some parts of the proof we use similar ideas as in [10, Lemma 2.3].

**Lemma 4.3.5.** *Let $\mu, \mu_0$ be defined in* (4.2.14)*. Then there exists a constant $C > 0$ such that for $N$ large enough we have*

$$0 < \mu - \mu_0 \leq O\left(\exp\left(-CN^{2\delta_L}\right)\right). \tag{4.3.16}$$

*Proof.* First we show that $\mu > \mu_0$. Remember that we certainly have $\mu < 4\pi^2$. In the following we denote $\Lambda_+^* := \Lambda^* \setminus \{0\}$. We use equation (4.2.14) to write

$$\begin{aligned}\sum_{p\in\Lambda_+^*} \frac{1}{\exp(\beta(p^2-\mu_0))-1} &= \mathrm{Tr}\left[\mathcal{N}\Gamma_{\mu_0}^0\right] = \mathrm{Tr}\left[\mathcal{N}\Gamma_\mu^{\mathrm{ec}}\right] \\ &= \sum_{p\in P_L\setminus\{0\}} \frac{1}{\exp(\beta(p^2-\mu))-1} < \sum_{p\in\Lambda_+^*} \frac{1}{\exp(\beta(p^2-\mu))-1}.\end{aligned} \tag{4.3.17}$$

As the map $x \mapsto (\exp(x)-1)^{-1}$, with $x > 0$, is monotonically decreasing inequality (4.3.17) implies $\mu > \mu_0$.
It remains to proof an upper bound. As a first step we quantify the effect of the energy cutoff on the particle number

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{N}\Gamma_\mu^{\mathrm{ec}}\right] &= \sum_{p\in P_L\setminus\{0\}} \frac{1}{\exp(\beta(p^2-\mu))-1} \\ &= \sum_{p\in\Lambda_+^*} \frac{1}{\exp(\beta(p^2-\mu))-1} - \sum_{p\in P_L^c} \frac{1}{\exp(\beta(p^2-\mu))-1} \\ &\geq \mathrm{Tr}\left[\mathcal{N}\Gamma_\mu^0\right] - C\exp\left(-cN^{2\delta_L}\right).\end{aligned} \tag{4.3.18}$$

In the last line we applied Lemma 4.3.3. By convexity of the map $x \mapsto (\exp(x)-1)^{-1}$ and the fact that $\exp(x)/(\exp(x)-1)^2 \geq 1/(\exp(x)-1)$ for $x > 0$ we have

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{N}\Gamma_\mu^0\right] - \mathrm{Tr}\left[\mathcal{N}\Gamma_{\mu_0}^0\right] &= \sum_{p\in\Lambda_+^*} \left[\frac{1}{\exp(\beta(p^2-\mu))-1} - \frac{1}{\exp(\beta(p^2-\mu_0))-1}\right] \\ &\geq \beta(\mu-\mu_0) \sum_{p\in\Lambda_+^*} \frac{\exp(\beta(p^2-\mu_0))}{\left(\exp(\beta(p^2-\mu_0))-1\right)^2} \\ &\geq \beta(\mu-\mu_0) \sum_{p\in\Lambda_+^*} \frac{1}{\exp(\beta(p^2-\mu_0))-1} \\ &= \beta N_{\mathrm{th}}(\mu-\mu_0).\end{aligned} \tag{4.3.19}$$

Using the bounds (4.3.18), (4.3.19) and our choice of chemical potentials (4.2.14) we get

$$\begin{aligned}0 = \mathrm{Tr}\left[\mathcal{N}\Gamma_\mu^{\mathrm{ec}}\right] - \mathrm{Tr}\left[\mathcal{N}\Gamma_{\mu_0}^0\right] &\geq \mathrm{Tr}\left[\mathcal{N}\Gamma_\mu^0\right] - \mathrm{Tr}\left[\mathcal{N}\Gamma_{\mu_0}^0\right] - C\exp\left(-cN^{2\delta_L}\right) \\ &\geq \beta N_{\mathrm{th}}(\mu-\mu_0) - C\exp\left(-cN^{2\delta_L}\right).\end{aligned}$$

This proves the claim. □

The following Lemma guarantees the existence of a pair $(\lambda_1, \lambda_2)$ such that (4.2.5) holds and quantifies the dependence of $\lambda_1$ and $\lambda_2$ on $g(N_0)$. We omit the proof here, it can be found in [8].

**Lemma 4.3.6.** *For $(\lambda_1, \lambda_2) \in \mathcal{D} = \{\mathbb{R} \times \mathbb{R} | \lambda_2 > 0\}$ we denote by p the distribution*

$$p(x) = Z^{-1}(\lambda_1, \lambda_2) \exp\Big( - \big(\lambda_1 x + \lambda_2 x^2\big)\Big) \tag{4.3.20}$$

*on $[0, \infty)$ with Z in* (4.2.4)*, and we choose $\mu_1, \mu_2 \in \mathbb{R}_+$ such that*

$$\mu_1^2 < \mu_2 < 2\mu_1^2 \tag{4.3.21}$$

*holds. Then there exists a pair $(\lambda_1, \lambda_2) \in \mathcal{D}$ such that the first two moments of p equal $\mu_1$ and $\mu_2$, respectively. Moreover, if we choose $\mu_1 = 1$ and $\mu_2 = 1 + g$ with $0 < g \ll 1$ then there exists a constant $c > 0$ such that*

$$\lambda_1 = -\frac{1}{g} + O\Big( \exp\big( - cg^{-1}\big)\Big) \quad \textit{and} \quad \lambda_2 = \frac{1}{2g} + O\Big( \exp\big( - cg^{-1}\big)\Big) \tag{4.3.22}$$

In our computations we will often need a rough estimate on the $L^1$-norm of the n-particle density matrix of $\tilde{\Gamma}_0$.

**Lemma 4.3.7.** *Let $\tilde{\Gamma}_0$ be the state defined in* (4.2.12)*, then we find for any $n \in \mathbb{N}_+$ a constant $C_n > 0$ independent of N such that*

$$\sum_{\substack{p_1,\dots,p_n \in \Lambda^* \\ q_1,\dots,q_n \in \Lambda^*}} \mathrm{Tr}\left[a^*_{p_1} \dots a^*_{p_n} a_{q_1} \dots a_{q_n} \tilde{\Gamma}_0\right] \leq C_n N^n. \tag{4.3.23}$$

*Proof.* We first need an estimate on the moments of the distribution $f$ with $(\lambda_1, \lambda_2) \in \mathcal{D}$ defined in (4.2.4). We claim that we find for any $n \in \mathbb{N}$ a constant $C_n > 0$ independent of $N_0$ such that

$$\int_0^\infty x^n f(x) dx \leq C_n N_0^n. \tag{4.3.24}$$

As the function $f$ has gaussian decay for large $x$ the integral on the r.h.s of (4.3.24) is certainly finite. We prove the claim by induction on $n$. The cases $0 \leq n \leq 2$ are given by Lemma 4.3.6. Assume that we have shown the inequality for $n \geq 2$. We write

$$\begin{aligned}
\int_0^\infty x^{n+1} f(x) dx &= \frac{N_0^{n+1}}{Z(\lambda_1, \lambda_2)} \int_0^\infty x^{n+1} \exp\Big( - \big(\lambda_1 x + \lambda_2 x^2\big)\Big) dx \\
&= -\frac{N_0^{n+1}}{2\lambda_2 Z(\lambda_1, \lambda_2)} \int_0^\infty x^n \frac{d}{dx}\Big( \exp\big( - \big(\lambda_1 x + \lambda_2 x^2\big)\big)\Big) dx \\
&\quad - \frac{\lambda_1 N_0^{n+1}}{2\lambda_2 Z(\lambda_1, \lambda_2)} \int_0^\infty x^n \exp\Big( - \big(\lambda_1 x + \lambda_2 x^2\big)\Big) dx \\
&= \frac{n N_0^{n+1}}{2\lambda_2 Z(\lambda_1, \lambda_2)} \int_0^\infty x^{n-1} \exp\Big( - \big(\lambda_1 x + \lambda_2 x^2\big)\Big) dx \\
&\quad - \frac{\lambda_1 N_0^{n+1}}{2\lambda_2 Z(\lambda_1, \lambda_2)} \int_0^\infty x^n \exp\Big( - \big(\lambda_1 x + \lambda_2 x^2\big)\Big) dx \\
&\leq \Big( C_{n-1} n g + C_n + O\Big( \exp\big( - cg^{-1}\big)\Big)\Big) N_0^{n+1}.
\end{aligned} \tag{4.3.25}$$

In the third equality we integrated by parts and in the last line we used (4.3.22) as well as the induction hypothesis. As we have $0 < g \ll 1$ the claim follows.
Applying the Wick theorem and Lemma 2.2.2 we can estimate for $n \in \mathbb{N}_+$

$$\begin{aligned}
&\sum_{\substack{p_1,\dots,p_n\in\Lambda^*\\ q_1,\dots,q_n\in\Lambda^*}} \mathrm{Tr}\left[a^*_{p_1}\dots a^*_{p_n}a_{q_1}\dots a_{q_n}\tilde{\Gamma}_0\right] \\
&\qquad = \sum_{j=0}^{n}\binom{n}{j}^2 \sum_{\substack{p_1,\dots,p_{n-j}\in\Lambda_+^*\\ q_1,\dots,q_{n-j}\in\Lambda_+^*}} \mathrm{Tr}\left[a^*_{p_1}\dots a^*_{p_{n-j}}a_{q_1}\dots a_{q_{n-j}}\Gamma^{\mathrm{ec}}_\mu\right]\int_{\mathbb{C}} f(|z|^2)\,\mathrm{Tr}\left[(a_0^*)^j(a_0)^j\,|z\rangle\langle z|\,\right]dz \\
&\qquad = \sum_{j=0}^{n}\binom{n}{j}^2 (n-j)!N_{\mathrm{th}}^{n-j}\int_{\mathbb{C}}|z|^{2j}f(|z|^2)dz \\
&\qquad = \sum_{j=0}^{n}\binom{n}{j}^2 (n-j)!N_{\mathrm{th}}^{n-j}\int_0^\infty x^j f(x)dx \\
&\qquad \le \sum_{j=0}^{n}\binom{n}{j}^2 (n-j)!N_{\mathrm{th}}^{n-j}C_jN_0^j \\
&\qquad \le C_nN^n. \qquad (4.3.26)
\end{aligned}$$

In the third equality we used (4.2.9) and in the first inequality we applied the bound (4.3.24). In the last inequality we used (4.2.18). □

When giving a bound for the entropy we will need an estimate for the effect of the correlation structure on the entropy. For this the following Lemma will be useful, which can be found in [23, Lemma 2].

**Lemma 4.3.8.** *Let $\Gamma = \sum_{\alpha=1}^\infty \lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ be a state, let $\{P_\alpha\}_{\alpha=1}^\infty$ be a family of one dimensional orthogonal projections, for which $P_\alpha P_\beta = \delta_{\alpha,\beta}$ need not hold, and define $\hat{\Gamma} = \sum_{\alpha=1}^\infty \lambda_\alpha P_\alpha$. Then*

$$S(\hat{\Gamma}) \ge S(\Gamma) - \ln\Big(\sum_{\alpha=1}^\infty \mathrm{Tr}\left[P_\alpha\hat{\Gamma}\right]\Big) \qquad (4.3.27)$$

*Proof.* Using the definition of $S$ we write

$$S(\hat{\Gamma}) - S(\Gamma) = -\sum_{\alpha=1}^\infty \lambda_\alpha \mathrm{Tr}\Big[P_\alpha \ln(\hat{\Gamma})\Big] + \sum_{\alpha=1}^\infty \lambda_\alpha \ln(\lambda_\alpha) = -\sum_{\alpha=1}^\infty \lambda_\alpha \mathrm{Tr}\Big[P_\alpha \ln\Big(\lambda_\alpha^{-1}\hat{\Gamma}\Big)\Big].$$

$\hat{\Gamma}$ is self-adjoint as the sum of everywhere defined orthogonal projections. Moreover, as $\hat{\Gamma}$ is trace-class it is also compact. Thus by the Hilbert-Schmidt Theorem we find a complete orthonormal basis $\{\phi_\beta\}_{\beta=1}^\infty$ of eigenvectors of $\hat{\Gamma}$. Using functional calculus we can write

$$\begin{aligned}
\mathrm{Tr}\Big[P_\alpha \ln\Big(\lambda_\alpha^{-1}\hat{\Gamma}\Big)\Big] &= \sum_{\beta=1}^\infty \langle\phi_\beta|P_\alpha\phi_\beta\rangle \ln\Big(\lambda_\alpha^{-1}\langle\phi_\beta|\hat{\Gamma}\phi_\beta\rangle\Big) \\
&\le \ln\Big(\sum_{\beta=1}^\infty \langle\phi_\beta|P_\alpha\phi_\beta\rangle\,\lambda_\alpha^{-1}\langle\phi_\beta|\hat{\Gamma}\phi_\beta\rangle\Big) = \ln\Big(\mathrm{Tr}\left[P_\alpha\lambda_\alpha^{-1}\hat{\Gamma}\right]\Big). \qquad (4.3.28)
\end{aligned}$$

In the inquality we used that $\mathrm{Tr}\,[P_\alpha] = 1$ and the concavity of the logarithm. Using the bound (4.3.28) and again the concavity of the logarithm we obtain

$$S(\hat{\Gamma}) - S(\Gamma) = -\sum_{\alpha=1}^{\infty} \lambda_\alpha \,\mathrm{Tr}\left[P_\alpha \ln\left(\lambda_\alpha^{-1}\hat{\Gamma}\right)\right] \geq -\sum_{\alpha=1}^{\infty} \lambda_\alpha \ln\Big(\mathrm{Tr}\,[P_\alpha \lambda_\alpha^{-1}\hat{\Gamma}]\Big) \geq -\ln\Big(\sum_{\alpha=1}^{\infty} \mathrm{Tr}\,[P_\alpha \hat{\Gamma}]\Big).$$

Reordering terms gives the desired bound. □

To derive the entropy contribution of the distribution over coherent condensate states, we will need a variant of the Berezin-Lieb inequality. The proof is adapted from Theorem A.1 in [25].

**Lemma 4.3.9.** *Let $p : [0,\infty) \to [0,\infty)$ be a probability distribution and $\xi : [0,\infty) \to [0,\infty)$ be a concave function. Define the operator*

$$A_p = \int_{\mathbb{C}} |z\rangle\langle z|\, p(|z|^2) dz \tag{4.3.29}$$

*on $\mathscr{F}_0$. Then we have*

$$\mathrm{Tr}\,[\xi(A_p)] \geq \int_0^\infty \xi(p(x)) dx. \tag{4.3.30}$$

*Proof.* From Lemma 2.2.2 we know that the projections $|z\rangle\langle z|$ for $z \in \mathbb{C}$ are self-adjoint and everywhere defined on the space $\mathscr{F}_0$. This and the fact that $p$ is a real-valued function implies that the operator $A_p$ is self-adjoint. As $A_p$ is trace-class it is also compact. Thus by the Hilbert-Schmidt Theorem we find a complete orthonormal basis $\{\psi_\alpha\}_{\alpha=1}^\infty$ of eigenvectors of $A_p$. By functional calculus we can write

$$\mathrm{Tr}\,[\xi(A_p)] = \sum_{\alpha=1}^{\infty} \xi\left(\int_{\mathbb{C}} \left|\langle z|\psi_\alpha\rangle\right|^2 p(|z|^2) dz\right). \tag{4.3.31}$$

Remember that $\int_{\mathbb{C}} |z\rangle\langle z|\, dz = 1_{\mathscr{F}_0}$. This implies that the function $z \mapsto \left|\langle z|\psi_\alpha\rangle\right|^2$ is a probability density on $\mathbb{C}$. As $p$ is a real-valued function, we are allowed to apply Jensen's inequality on the r.h.s of (4.3.31)

$$\mathrm{Tr}\,[\xi(A_p)] \geq \sum_{\alpha=1}^{\infty} \int_{\mathbb{C}} |\langle z|\psi_\alpha\rangle|^2 \xi\Big(p(|z|^2)\Big) dz.$$

As $|z\rangle\langle z|$ is a one-dimensional projection for any $z \in \mathbb{C}$ we have $\sum_{\alpha=1}^\infty \left|\langle z|\psi_\alpha\rangle\right|^2 = 1$. Using this equality after exchanging the integral with the sum (which is allowed because $\xi \geq 0$) and performing a change of variables as it is done in (4.2.9) we obtain

$$\mathrm{Tr}\,[\xi(A_p)] \geq \int_{\mathbb{C}} \xi\Big(p(|z|^2)\Big) dz = \int_0^\infty \xi\Big(p(x)\Big) dx.$$

□

## 4.4 Particle Expectation of the Trial State

In this section we prove the estimate (4.2.17). Let $1 \leq \alpha < \infty$ and notice that we have the trivial lower bound

$$\langle (1+\eta)\psi_\alpha | (1+\eta)\psi_\alpha \rangle = 1 + 2\mathrm{Re}(\langle \psi_\alpha | \eta\psi_\alpha \rangle) + \langle \eta\psi_\alpha | \eta\psi_\alpha \rangle = 1 + \langle \eta\psi_\alpha | \eta\psi_\alpha \rangle \geq 1. \tag{4.4.1}$$

Here we used that $\psi_\alpha$ does not contain momenta $p$ such that $|p| \geq N^{1-\delta_H} > N^{1/3+\delta_L}$.
Moreover we have for the expected number of particles of $\tilde{\Gamma}_0$:

$$\begin{aligned}\mathrm{Tr}\,[\mathcal{N}\tilde{\Gamma}_0] &= \int_{\mathbb{C}} f(|z|^2)\,\mathrm{Tr}\left[a_0^* a_0 \,|z\rangle\langle z|\,\right]dz + \mathrm{Tr}\left[\sum_{p\in\Lambda_+^*} a_p^* a_p \Gamma_\mu^{\mathrm{ec}}\right] \\ &= \int_{\mathbb{C}} f(|z|^2)|z|^2 dz + N_{\mathrm{th}} = \int_0^\infty x f(x)dx + N_{\mathrm{th}} = N_0 + N_{\mathrm{th}}.\end{aligned}$$

Here we used the definition of the chemical potential $\mu$ in (4.2.14) and Lemma 2.2.2 in the second equality. In the third equality we used equation (4.2.9).
To obtain an upper bound for the particle expectation of the trial state we write

$$\begin{aligned}\mathrm{Tr}[\mathcal{N}\Gamma] = \sum_{\alpha=1}^\infty \lambda_\alpha \frac{\langle (1+\eta)\psi_\alpha \big| \mathcal{N}(1+\eta)\psi_\alpha\rangle}{\langle (1+\eta)\psi_\alpha \big| (1+\eta)\psi_\alpha\rangle} &\leq \sum_{\alpha=1}^\infty \lambda_\alpha \langle \psi_\alpha \big| \mathcal{N}\psi_\alpha\rangle + \sum_{\alpha=1}^\infty \lambda_\alpha \langle \eta\psi_\alpha \big| \mathcal{N}\eta\psi_\alpha\rangle \\ &= N_0 + N_{\mathrm{th}} + \mathrm{Tr}\,[\eta^* \mathcal{N}\eta\tilde{\Gamma}_0].\end{aligned} \tag{4.4.2}$$

For the second term in (4.4.2) we estimate

$$\begin{aligned}\mathrm{Tr}\,[\eta^*\mathcal{N}\eta\tilde{\Gamma}_0] &= \frac{1}{4N^2} \sum_{\substack{p\in\Lambda^*, p_1,p_2\in P_H \\ u_1,v_1,u_2,v_2\in P_L}} \eta_{p_1}\eta_{p_2}\,\mathrm{Tr}\,[a_{u_1}^* a_{v_1}^* a_{u_1+p_1} a_{v_1-p_1} a_p^* a_p a_{u_2+p_2}^* a_{v_2-p_2}^* a_{u_2} a_{v_2}\tilde{\Gamma}_0] \\ &\leq \frac{C}{N^2} \sum_{\substack{p\in\Lambda^*, p_1,p_2\in P_H \\ u_1,v_1,u_2,v_2\in P_L}} |\eta_{p_1}\eta_{p_2}|\,\mathrm{Tr}\,[a_{u_1}^* a_{v_1}^* a_p^* a_p a_{u_2} a_{v_2}\tilde{\Gamma}_0] \\ &\qquad \cdot \left(\delta_{u_1+p_1,u_2+p_2}\delta_{v_1-p_1,v_2-p_2} + \delta_{u_1+p_1,v_2-p_2}\delta_{u_1+p_1,v_2-p_2}\right) \\ &\leq \frac{C}{N^2}\|\eta\|_{L^2(P_H)}^2 \sum_{\substack{p\in\Lambda^* \\ u_1,v_1,u_2,v_2\in P_L}} \mathrm{Tr}\,[a_{u_1}^* a_{v_1}^* a_p^* a_p a_{u_2} a_{v_2}\tilde{\Gamma}_0] \\ &\leq CN^{\delta_H+2\kappa}.\end{aligned} \tag{4.4.3}$$

In the first inequality we used that $\tilde{\Gamma}_0$ does not contain momenta in $P_L^c$, thus $a_{u_1+p_1}$, $a_{v_1-p_1}$ contracted with $a_{u_2+p_2}^*$, $a_{v_2-p_2}^*$ give the biggest nonzero contributions. There is also the possibility to contract some of them with $a_p^*$, $a_p$ but it is not difficult to see that these terms are smaller. Thus, the contractions $a_{u_1+p_1}$, $a_{v_1-p_1}$ with $a_{u_2+p_2}^*$, $a_{v_2-p_2}^*$ multiplied with a constant large enough is an appropriate upper bound.
The second inequality follows by an application of Cauchy-Schwarz:

$$\max_{u\in 2P_L} \sum_{p\in P_H} |\eta_p\eta_{p+u}|\chi(p+u\in P_H) \leq \max_{u\in 2P_L}\left(\sum_{p\in P_H}|\eta_{p+u}|^2\chi(p+u\in P_H)\right)^{1/2}\left(\sum_{p\in P_H}|\eta_p|^2\right)^{1/2} \leq \|\eta\|_{L^2(P_H)}^2.$$

From now on we just refer to the Cauchy-Schwarz inequality for estimates similar to the second inequality of (4.4.3). In the last inequality of (4.4.3) we used Lemma 4.3.2 and Lemma 4.3.7. In combination, (4.4.2) and (4.4.3) imply

$$\mathrm{Tr}[\mathcal{N}\Gamma] \leq N_0 + N_{\mathrm{th}} + CN^{\delta_H+2\kappa}. \tag{4.4.4}$$

Define the operators $\mathcal{N}_0 := a_0^* a_0$, $\mathcal{N}_> := \sum_{p\in\Lambda^*\setminus\{0\}} a_p^* a_p$ and let $c > 3$. For the lower bound we write

$$\begin{aligned}
\mathrm{Tr}[\mathcal{N}\Gamma] &= \sum_{\alpha=1}^{\infty} \lambda_\alpha \frac{\langle (1+\eta)\psi_\alpha \big| \mathcal{N}(1+\eta)\psi_\alpha\rangle}{\langle (1+\eta)\psi_\alpha \big| (1+\eta)\psi_\alpha\rangle} \geq \sum_{\alpha=1}^{\infty} \lambda_\alpha \frac{\langle \psi_\alpha \big| \mathcal{N}\chi(\mathcal{N}_0 \leq cN)\chi(\mathcal{N}_> \leq cN)\psi_\alpha\rangle}{1+\langle \eta\psi_\alpha \big| \eta\psi_\alpha\rangle} \\
&\geq \sum_{\alpha=1}^{\infty} \lambda_\alpha \langle \psi_\alpha \big| \mathcal{N}\chi(\mathcal{N}_0 \leq cN)\chi(\mathcal{N}_> \leq cN)\psi_\alpha\rangle \Big(1 - \langle \eta\psi_\alpha \big| \eta\psi_\alpha\rangle\Big) \\
&\geq \mathrm{Tr}\left[\mathcal{N}\chi(\mathcal{N}_0 \leq cN)\chi(\mathcal{N}_> \leq cN)\tilde{\Gamma}_0\right] - 2cN\,\mathrm{Tr}\left[\eta^*\eta\tilde{\Gamma}_0\right] \\
&\geq \mathrm{Tr}\left[\mathcal{N}\tilde{\Gamma}_0\right] - CN^{\delta_H+2\kappa} + \mathrm{Tr}\left[\mathcal{N}(\chi(\mathcal{N}_0 \leq cN)\chi(\mathcal{N}_> \leq cN) - 1)\tilde{\Gamma}_0\right] \\
&= N_0 + N_{\mathrm{th}} - CN^{\delta_H+2\kappa} - \mathrm{Tr}\left[\mathcal{N}(\chi(\mathcal{N}_0 > cN)\chi(\mathcal{N}_> \leq cN) + \chi(\mathcal{N}_> > cN))\tilde{\Gamma}_0\right].
\end{aligned} \tag{4.4.5}$$

In the fourth inequality we used the bound

$$\mathrm{Tr}\left[\eta^*\eta\tilde{\Gamma}_0\right] \leq CN^{-1+\delta_H+2\kappa}, \tag{4.4.6}$$

which is derived with similar arguments as used in (4.4.3). It remains to give an estimation to the last term in (4.4.5). To this end we write

$$\begin{aligned}
\mathrm{Tr}\left[\mathcal{N}(\chi(\mathcal{N}_0 > cN)\chi(\mathcal{N}_> \leq cN) + \chi(\mathcal{N}_> > cN))\tilde{\Gamma}_0\right] &\leq \mathrm{Tr}\left[(\mathcal{N}_0 + \mathcal{N}_>)(\chi(\mathcal{N}_0 > cN) + \chi(\mathcal{N}_> > cN))\tilde{\Gamma}_0\right] \\
&= \int_{\mathbb{C}} \mathrm{Tr}\left[\mathcal{N}_0\chi(\mathcal{N}_0 > cN)\,|z\rangle\langle z|\,\right] f(|z|^2)dz + N_{\mathrm{th}} \int_{\mathbb{C}} \mathrm{Tr}\left[\chi(\mathcal{N}_0 > cN)\,|z\rangle\langle z|\,\right] f(|z|^2)dz \\
&\quad + \mathrm{Tr}\left[\mathcal{N}_>\chi(\mathcal{N}_> > cN)\tilde{\Gamma}_\mu^{\mathrm{ec}}\right] + N_0\,\mathrm{Tr}\left[\chi(\mathcal{N}_> > cN)\tilde{\Gamma}_\mu^{\mathrm{ec}}\right].
\end{aligned} \tag{4.4.7}$$

For computational convenience we assume in the following that $g = CN_0^{-\varepsilon}$ where $0 < \varepsilon < 1$. In section 4.8 we see that the optimal $g$ fulfills this condition. Note that $\{1^{\otimes n}\}_{n=0}^{\infty}$ is an orthonormal basis of $\mathscr{F}_0$ consisting of eigenfunctions of $\mathcal{N}_0$. Thus, for the first terms on the r.h.s of (4.4.7) we can write using Lemma 2.2.1:

$$\begin{aligned}
&\int_{\mathbb{C}} \mathrm{Tr}\left[\mathcal{N}_0\chi(\mathcal{N}_0 > cN)\,|z\rangle\langle z|\,\right] f(|z|^2)dz = \sum_{n>cN} n \int_{\mathbb{C}} |\langle 1^{\otimes n}|z\rangle|^2 f(|z|^2)dz \\
&= \sum_{n>cN} n \int_{\mathbb{C}} \frac{|z|^{2n}}{n!} \exp(-|z|^2) f(|z|^2)dz \\
&= N_0^{-1} Z(\lambda_1,\lambda_2)^{-1} \sum_{n>cN} n \int_0^{\infty} \frac{x^n}{n!} \exp\Big(-\Big(x + \lambda_1 N_0^{-1}x + \lambda_2 N_0^{-2}x^2\Big)\Big)dx \\
&= N_0^{-1} Z(\lambda_1,\lambda_2)^{-1} \sum_{n>cN} n \int_0^{\infty} \frac{x^n}{n!} \exp\Big(-\Big(1 + (gN_0)^{-1}\Big)x - \Big((\lambda_1 N_0^{-1} - (gN_0)^{-1})x + \lambda_2 N_0^{-2}x^2\Big)\Big)dx \\
&\leq N_0^{-1} Z(\lambda_1,\lambda_2)^{-1} \exp\Big(\frac{(\lambda_1 - g^{-1})^2}{4\lambda_2}\Big) \sum_{n>cN} n \int_0^{\infty} \frac{x^n}{n!} \exp\Big(-\Big(1 + (gN_0)^{-1}\Big)x\Big)\Big)dx \\
&= N_0^{-1} Z(\lambda_1,\lambda_2)^{-1} \exp\Big(\frac{(\lambda_1 - g^{-1})^2}{4\lambda_2}\Big) \sum_{n>cN} \frac{n}{\left(1 + (gN_0)^{-1}\right)^{n+1}}.
\end{aligned} \tag{4.4.8}$$

In the first inequality we used that the function $x \mapsto (\lambda_1 N_0^{-1} - (gN_0)^{-1})x + \lambda_2 N_0^{-2} x^2$ attains its minimum at $x = (g^{-1} - \lambda_1)N_0(2\lambda_2)^{-1}$. The last equality follows by $n$-times partial integration. Notice that we have

$$Z(\lambda_1, \lambda_2) = \int_0^\infty \exp\Big( - \big(\lambda_1 x + \lambda_2 x^2\big)\Big) dx = \frac{\exp\left(\frac{\lambda_1^2}{4\lambda_2}\right)}{(2\lambda_2)^{1/2}} \int_{\frac{\lambda_1}{\sqrt{2\lambda_2}}}^\infty \exp\left(-\frac{x^2}{2}\right) dx \geq C\lambda_2^{-1/2} \exp\left(\frac{\lambda_1^2}{4\lambda_2}\right), \tag{4.4.9}$$

where we applied Lemma 4.3.6 to see that $\lambda_1(2\lambda_2)^{-1/2} < 0$. Assume w.l.o.g that $cN \in \mathbb{N}$. In this case we compute for the sum on the r.h.s of (4.4.8):

$$\begin{aligned} \sum_{n>cN} \frac{n}{(1 + (gN_0)^{-1})^{n+1}} &= -\frac{\partial}{\partial x}\left(\sum_{n>cN} x^{-n}\right)\Big|_{x=1+(gN_0)^{-1}} = -\frac{\partial}{\partial x}\left(\frac{x^{-(cN+1)}}{1 - x^{-1}}\right)\Big|_{x=1+(gN_0)^{-1}} \\ &= \Big(1 + (gN_0)^{-1}\Big)^{-(cN+1)} (cN + 1 + gN_0) gN_0 \leq CNgN_0 \Big(1 + (gN_0)^{-1}\Big)^{-(cN+1)}. \end{aligned} \tag{4.4.10}$$

Considering (4.4.9), (4.4.10) and an application of Lemma 4.3.6 yields

$$\begin{aligned} N_0^{-1} Z(\lambda_1, \lambda_2)^{-1} \exp\Big(\frac{(\lambda_1 - g^{-1})^2}{4\lambda_2}\Big) &\sum_{n>cN} \frac{n}{(1 + (gN_0)^{-1})^{n+1}} \\ &\leq C\lambda_2^{1/2} Ng \exp\Big( - \frac{\lambda_1 g^{-1}}{2\lambda_2} + \frac{g^{-2}}{4\lambda_2}\Big)\Big(1 + (gN_0)^{-1}\Big)^{-(cN+1)} \\ &\leq Cg^{1/2} N \exp\Big(3/2g^{-1}\Big)\Big(1 + (gN_0)^{-1}\Big)^{-cN_0} \\ &\leq Cg^{1/2} N \exp\Big( - (c-3)/2g^{-1}\Big). \end{aligned} \tag{4.4.11}$$

The last inequality follows from the estimate

$$\begin{aligned} \Big(1 + (gN_0)^{-1}\Big)^{-cN_0} &= \exp\Big( - cN_0 \ln\Big(1 + (gN_0)^{-1}\Big)\Big) \leq \exp\Big( - cN_0\Big((gN_0)^{-1} - (gN_0)^{-2}/2\Big)\Big) \\ &\leq \exp\Big( - cg^{-1}\Big(1 - (gN_0)^{-1}/2\Big)\Big) \leq \exp\Big( - cg^{-1}/2\Big), \end{aligned}$$

where we used the bound $\ln(1 + x) \geq x - x^2/2$ for $0 \leq x < 1/2$ and the fact that $(gN_0)^{-1} \to 0$ for $N \to \infty$ which is implied by $g = CN_0^{-\varepsilon}$ where $0 < \varepsilon < 1$. Thus, we find a constant $c_1 > 0$ s.t. we have the following estimate for the first term on the r.h.s of (4.4.7):

$$\int_{\mathbb{C}} \mathrm{Tr}\left[\mathcal{N}_0 \chi(\mathcal{N}_0 > cN) \left|z\right\rangle \left\langle z\right| \right] f(|z|^2) dz \leq C \exp\Big( - c_1 N^\varepsilon\Big).$$

Here we used the assumption $\beta \geq \beta_c(1 + \delta)$ for some $\delta > 0$ and that $c > 3$. The second term on the r.h.s of (4.4.7) can be bounded in a similar way. The third and fourth term on the r.h.s of (4.4.7) are estimated by an application of Lemma 4.3.4. All together we find $p > 0$ and $c_2 > 0$ s.t. we have

$$\mathrm{Tr}\left[\mathcal{N}(\chi(\mathcal{N}_0 > cN)\chi(\mathcal{N}_> \leq cN) + \chi(\mathcal{N}_> > cN))\tilde{\Gamma}_0\right] \leq C \exp\Big( - c_2 N^p\Big).$$

Together with (4.4.5) this gives us the lower bound

$$\mathrm{Tr}[\mathcal{N}\Gamma] \geq N_0 + N_{\mathrm{th}} - CN^{\delta_H + 2\kappa}. \tag{4.4.12}$$

## 4.5 Estimation of the Energy

The goal of this section is to give a bound for the energy expectation $\mathrm{Tr}\,[H_N\Gamma]$.
We would like to exploit the fact that $\{\psi_\alpha\}_{\alpha=1}^\infty$ are chosen to be eigenfunctions of $H_0$ on $\mathcal{F}_>$ with eigenvalues $\{E_\alpha\}_{\alpha=1}^\infty$. Thus we have to commute the kinetic energy operator $H_0$ with the correlation operator $(1+\eta)$ which gives

$$\begin{aligned}
\mathrm{Tr}\,[H_N\Gamma] &= \sum_\alpha \lambda_\alpha \frac{\langle (1+\eta)\psi_\alpha \big| (H_0+\mathcal{V}_N)(1+\eta)\psi_\alpha\rangle}{\langle (1+\eta)\psi_\alpha \big| (1+\eta)\psi_\alpha\rangle} \\
&= \sum_\alpha \lambda_\alpha \frac{\langle (1+\eta)\psi_\alpha \big| (1+\eta)H_0\psi_\alpha\rangle}{\langle (1+\eta)\psi_\alpha \big| (1+\eta)\psi_\alpha\rangle} + \sum_\alpha \lambda_\alpha \frac{\langle (1+\eta)\psi_\alpha \big| ([H_0,\eta]+\mathcal{V}_N(1+\eta))\psi_\alpha\rangle}{\langle (1+\eta)\psi_\alpha \big| (1+\eta)\psi_\alpha\rangle} \\
&\leq \sum_\alpha \lambda_\alpha E_\alpha + \Big| \sum_\alpha \lambda_\alpha \langle (1+\eta)\psi_\alpha \big| ([H_0,\eta]+\mathcal{V}_N(1+\eta))\psi_\alpha\rangle \Big| \\
&= \mathrm{Tr}[H_0\tilde{\Gamma}_0] + \Big| \mathrm{Tr}\Big[(1+\eta^*)\Big([H_0,\eta]+\mathcal{V}_N(1+\eta)\Big)\tilde{\Gamma}_0\Big]\Big|, \qquad (4.5.1)
\end{aligned}$$

where we used the bound (4.4.1) in the inequality. Using the canonical commutation relations (4.2.2) the commutator $[H_0,\eta]$ can be written as

$$\begin{aligned}
[H_0,\eta] &= \frac{1}{2N} \sum_{\substack{p_1\in\Lambda^*, p_2\in P_H \\ u,v\in P_L}} p_1^2 \eta_{p_2} [a^*_{p_1}a_{p_1}, a^*_{u+p_2}a^*_{v-p_2}a_u a_v] \\
&= \frac{1}{2N} \sum_{\substack{p_1\in\Lambda^*, p_2\in P_H \\ u,v\in P_L}} p_1^2 \eta_{p_2} \Big( a^*_{p_1}[a_{p_1}, a^*_{u+p_2}a^*_{v-p_2}a_u a_v] + [a^*_{p_1}, a^*_{u+p_2}a^*_{v-p_2}a_u a_v]a_{p_1}\Big) \\
&= \frac{1}{2N} \sum_{\substack{p_1\in\Lambda^*, p_2\in P_H \\ u,v\in P_L}} p_1^2 \eta_{p_2} \\
&\qquad \cdot \Big( a^*_{p_1}\Big([a_{p_1}, a^*_{u+p_2}]a^*_{v-p_2} + a^*_{u+p_2}[a_{p_1}, a^*_{v-p_2}]\Big)a_u a_v + a^*_{u+p_2}a^*_{v-p_2}\Big([a^*_{p_1}, a_u]a_v + a_u[a^*_{p_1}, a_v]\Big)a_{p_1}\Big) \\
&= \frac{1}{2N} \sum_{p\in P_H, u,v\in P_L} \eta_p \left[(u+p)^2 + (v-p)^2 - u^2 - v^2\right] a^*_{u+p}a^*_{v-p}a_u a_v \\
&= \frac{1}{N} \sum_{p\in P_H, u,v\in P_L} \eta_p p^2 a^*_{u+p}a^*_{v-p}a_u a_v + \frac{1}{N} \sum_{p\in P_H, u,v\in P_L} \eta_p p\cdot(u-v) a^*_{u+p}a^*_{v-p}a_u a_v \\
&:= \mathcal{K} + \mathcal{K}_L. \qquad (4.5.2)
\end{aligned}$$

The rest of this section is devoted to estimating the second term in (4.5.1). We write

$$\begin{aligned}
&\mathrm{Tr}\Big[(1+\eta^*)\Big([H_0,\eta]+\mathcal{V}_N(1+\eta)\Big)\tilde{\Gamma}_0\Big] \\
&\qquad = \mathrm{Tr}\Big[\mathcal{V}_N(1+\eta)\tilde{\Gamma}_0\Big] + \mathrm{Tr}\Big[\eta^*(\mathcal{K}+\mathcal{V}_N)\tilde{\Gamma}_0\Big] + \mathrm{Tr}\Big[\eta^*\mathcal{V}_N\eta\tilde{\Gamma}_0\Big] + \mathrm{Tr}\Big[(\mathcal{K}+(1+\eta^*)\mathcal{K}_L)\tilde{\Gamma}_0\Big]. \qquad (4.5.3)
\end{aligned}$$

### 4.5.1 Interaction Energy

The first term on the r.h.s of (4.5.3) can be written as

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{V}_N(1+\eta)\tilde{\Gamma}_0\right] &= \frac{1}{2N^{1-\kappa}}\sum_{p,u,v\in\Lambda^*}\hat{V}(p/N^{1-\kappa})\,\mathrm{Tr}\left[a^*_{u+p}a^*_{v-p}a_ua_v\tilde{\Gamma}_0\right]\\ &\quad+\frac{1}{4N^{2-\kappa}}\sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in P_H,u_2,v_2\in P_L}}\hat{V}(p_1/N^{1-\kappa})\eta_{p_2}\,\mathrm{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_1}a_{v_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right].\end{aligned} \tag{4.5.4}$$

As $u+p\notin P_L$ for $u\in P_L$ and $p\in P_H$, we see that in the second term of (4.5.4) only commutators containing $a^*_{u_2+p_2}, a^*_{v_2-p_2}$ give non-zero contributions. This is due to the energy cutoff. There are two possible combinations of commutators. After redefining $p_1\to -p_1$ for one of these combinations, we see that they are actually the same due to the radial symmetry of $P_H$ and $\hat{V}(p)$. Thus the second term on the r.h.s of (4.5.4) is equal to

$$\begin{aligned}&\frac{1}{2N^{2-\kappa}}\sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in P_H,u_2,v_2\in P_L}}\hat{V}(p_1/N^{1-\kappa})\eta_{p_2}\,\mathrm{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\delta_{u_1,u_2+p_2}\delta_{v_1,v_2-p_2}\\ &\qquad=\frac{1}{2N^{4-4\kappa}}\sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in\Lambda^*,u_2,v_2\in P_L}}\hat{V}(p_1/N^{1-\kappa})\hat{f}_\ell(p_2/N^{1-\kappa})\,\mathrm{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\delta_{u_1,u_2+p_2}\delta_{v_1,v_2-p_2}\end{aligned} \tag{4.5.5}$$

$$-\frac{1}{2N^{1-\kappa}}\sum_{p_1\in\Lambda^*,u_1,v_1\in P_L}\hat{V}(p_1/N^{1-\kappa})\,\mathrm{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_1}a_{v_1}\tilde{\Gamma}_0\right] \tag{4.5.6}$$

$$-\frac{1}{2N^{2-\kappa}}\sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in P_H^c,u_2,v_2\in P_L}}\hat{V}(p_1/N^{1-\kappa})\eta_{p_2}\,\mathrm{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\delta_{u_1,u_2+p_2}\delta_{v_1,v_2-p_2}. \tag{4.5.7}$$

Here we used that

$$\eta_p=-\frac{N^\kappa}{N^{2-2\kappa}}\widehat{(1-f_\ell(\cdot))}(p/N^{1-\kappa})=-N\delta_{p,0}+\frac{N^\kappa}{N^{2-2\kappa}}\hat{f}_\ell(p/N^{1-\kappa}).$$

The term (4.5.6) cancels with the first term in (4.5.4). To see this, we notice that due to the momentum cutoff in $\tilde{\Gamma}_0$ we have for the remaining term

$$\frac{1}{2N^{1-\kappa}}\sum_{\substack{p\in\Lambda^*\\ (u,v)\in(P_L\times P_L)^c}}\hat{V}(p/N^{1-\kappa})\,\mathrm{Tr}[a^*_{u+p}a^*_{v-p}a_ua_v\tilde{\Gamma}_0]=0.$$

Let us derive a bound for the term (4.5.7). As the potential $V$ is compactly supported and $V \in L^3(\mathbb{R}^3)$ we have $V \in L^1(\mathbb{R}^3)$ which implies $\|\hat{V}\|_\infty < \infty$. Using this fact, Lemma 4.3.7 and 2.5.1 we can write

$$\begin{aligned}
&\frac{1}{2N^{2-\kappa}} \sum_{\substack{p_1,u_1,v_1\in\Lambda^* \\ p_2\in P_H^c, u_2,v_2\in P_L}} \hat{V}(p_1/N^{1-\kappa})\eta_{p_2} \operatorname{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\delta_{u_1,u_2+p_2}\delta_{v_1,v_2-p_2} \\
&\qquad \leq \frac{1}{2N^{2-\kappa}} \sum_{p_2\in P_H^c} \left|\eta_{p_2}\right| \left( \sum_{p_1\in\Lambda^*, u_2,v_2\in P_L} \operatorname{Tr}\left[a^*_{u_2+p_2+p_1}a^*_{v_2-p_2-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\right) \\
&\qquad \leq CN^{\kappa} \sum_{p_2\in P_H^c} \left|\eta_{p_2}\right| \leq CN^{2\kappa} \int_{\{|p|\leq N^{1-\delta_H}\}} \frac{1}{|p|^2} dp \\
&\qquad \leq CN^{1-\delta_H+2\kappa}.
\end{aligned}$$

It remains to estimate the term (4.5.5). To do this, we need the following bound

$$\begin{aligned}
\left|\sum_{p\in\Lambda^*} \hat{V}((p+u)/N^{1-\kappa})\hat{f}_N(p/N^{1-\kappa})\right| &= N^{6-6\kappa}\left|\int V(N^{1-\kappa}x)e^{-ix\cdot u}f_\ell(N^{1-\kappa}x)dx\right| \\
&\leq N^{3-3\kappa}\int V(x)f_\ell(x)dx \leq N^{3-3\kappa}\left(8\pi a + \frac{Ca^2}{N^{1-\kappa}\ell}\right), \qquad (4.5.8)
\end{aligned}$$

where $u \in \Lambda^*$. Here we used Plancherel's Theorem (see Theorem 5.3. in [16]) in the first line, $f \geq 0$ and $V \geq 0$ in the second line and applied Lemma 2.5.1 in the third line.
Using this estimate we can write for (4.5.5)

$$\begin{aligned}
&\frac{1}{2N^{4-4\kappa}} \sum_{\substack{p_1,u_1,v_1\in\Lambda^* \\ p_2\in\Lambda^*, u_2,v_2\in P_L}} \hat{V}(p_1/N^{1-\kappa})\hat{f}_\ell(p_2/N^{1-\kappa}) \operatorname{Tr}\left[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\delta_{u_1,u_2+p_2}\delta_{v_1,v_2-p_2} \\
&\quad = \frac{1}{2N^{4-4\kappa}} \sum_{p_1,p_2\in\Lambda^*} \hat{V}(p_1/N^{1-\kappa})\hat{f}_\ell(p_2/N^{1-\kappa}) \left( \sum_{u_2,v_2\in P_L} \operatorname{Tr}\left[a^*_{u_2+p_2+p_1}a^*_{v_2-p_2-p_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right]\right) \\
&\quad = \frac{1}{2N^{4-4\kappa}} \sum_{p_1,p_2\in\Lambda^*} \hat{V}(p_1/N^{1-\kappa})\hat{f}_\ell(p_2/N^{1-\kappa}) \\
&\qquad \int_{\mathbb{C}} f(|z|^2)\Big(\delta_{p_1+p_2,0}|z|^4 + 2|z|^2 \sum_{u_2\in P_L\setminus\{0\}} \hat{\gamma}_0(u_2)\left(\delta_{p_1+p_2,0} + \delta_{u_2+p_1+p_2,0}\right) \\
&\qquad\quad + \sum_{u_2,v_2\in P_L\setminus\{0\}} \hat{\gamma}_0(u_2)\hat{\gamma}_0(v_2)\left(\delta_{p_2+p_1,0} + \delta_{u_2+p_2+p_1,v_2}\right)\Big)dz \\
&\quad \leq \frac{1}{2N^{1-\kappa}}\left(8\pi a + \frac{Ca^2}{N^{1-\kappa}\ell}\right) \int_{\mathbb{C}} f(|z|^2)\left(|z|^4 + 4|z|^2 \sum_{u_2\in P_L\setminus\{0\}} \hat{\gamma}_0(u_2) + 2 \sum_{u_2,v_2\in P_L\setminus\{0\}} \hat{\gamma}_0(u_2)\hat{\gamma}_0(v_2)\right)dz \\
&\quad \leq \frac{1}{2N^{1-\kappa}}\left(8\pi a + \frac{Ca^2}{N^{1-\kappa}\ell}\right)\left(N_0^2(1+g(N_0)) + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\right) \\
&\quad \leq \frac{1}{N^{1-\kappa}} 4\pi a\left(N_0^2(1+g(N_0)) + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\right) + CN^{2\kappa}.
\end{aligned}$$

In the second equality we applied the Wick theorem and used Lemma 2.2.2 which implies $W^*_{N_0}a_pW_{N_0} = a_p + z\delta_{p,0}$ and $W^*_{N_0}a^*_pW_{N_0} = a_p + \bar{z}\delta_{p,0}$. In the first inequality we exchanged sums, exploited the radial

symmetry of $\hat{V}, \hat{f}_\ell$ and used the bound (4.5.8). In the second inequality we used (4.2.5) and (4.2.9). In combination, the above considerations show that the first term in (4.5.3) is bounded from above by

$$\mathrm{Tr}\,[\mathcal{V}_N(1+\eta)\tilde{\Gamma}_0] \leq \frac{1}{N^{1-\kappa}} 4\pi a \Big( N_0^2(1+g(N_0)) + 4N_0 N_{\mathrm{th}} + 2N_{\mathrm{th}}^2 \Big) + CN^{1-\delta_H+2\kappa}. \tag{4.5.9}$$

## 4.5.2 Application of the Scattering Equation

The scattering equation provides us with a convenient way to cancel terms. In this subsection we see how we can apply it to the second term on the r.h.s of (4.5.3).
As seen for the term (4.5.4), we can argue that commutators containing $a_{u_1+p_1}, a_{v_1-p_1}$ give the only non-zero contributions. Thus the second term on the r.h.s of (4.5.3) is equal to

$$\frac{1}{N^2} \sum_{\substack{p_1,p_2\in P_H \\ u_1,u_2,v_1,v_2\in P_L}} \eta_{p_1} \left( \frac{N^\kappa}{2} \hat{V}(p_2/N^{1-\kappa}) + p_2^2 \eta_{p_2} \right) \mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1,u_2+p_2} \delta_{v_1-p_1,v_2-p_2} \tag{4.5.10}$$

$$+ \frac{1}{2N^{2-\kappa}} \sum_{\substack{p_1\in P_H u_1,v_1\in P_L \\ (p_2,u_2,v_2)\in (P_H\times P_L\times P_L)^c}} \eta_{p_1} \hat{V}(p_2/N^{1-\kappa}) \,\mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1,u_2+p_2} \delta_{v_1-p_1,v_2-p_2}. \tag{4.5.11}$$

A factor $1/2$ canceled out because we have two possibilities of contracting $a_{u_1+p_1}, a_{v_1-p_1}$ and after redefining $p_1 \to -p_1$ we see that they are the same.
We can apply the scattering equation (2.5.13) to the first term above and get

$$\begin{aligned} &\frac{1}{N^2} \sum_{\substack{p_1,p_2\in P_H \\ u_1,u_2,v_1,v_2\in P_L}} \eta_{p_1} \left( \frac{N^\kappa}{2} \hat{V}(p_2/N^{1-\kappa}) + p_2^2 \eta_{p_2} \right) \mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1,u_2+p_2} \delta_{v_1-p_1,v_2-p_2} \\ &= \frac{1}{N^2} \sum_{\substack{p_1,p_2\in P_H \\ u_1,u_2,v_1,v_2\in P_L}} \eta_{p_1} N^{3-2\kappa} \lambda_l (\hat{\chi}_\ell * \hat{f}_N)(p_2) \,\mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1,u_2+p_2} \delta_{v_1-p_1,v_2-p_2} \end{aligned} \tag{4.5.12}$$

$$- \frac{1}{N^2} \sum_{\substack{p_1,p_2\in P_H \\ u_1,u_2,v_1,v_2\in P_L}} \eta_{p_1} \left( \frac{1}{2N} \sum_{q\in\Lambda^*} N^\kappa \hat{V}((p_2-q)/N^{1-\kappa}) \eta_q \right) \mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1,u_2+p_2} \delta_{v_1-p_1,v_2-p_2}. \tag{4.5.13}$$

Term 4.5.12 can be bounded using Lemma 4.3.7, Lemma 2.5.1 $\Big($which implies $\big|N^{3-2\kappa}\lambda_\ell\big| \leq C\frac{N^\kappa a}{\ell^3} + C\frac{N^{-1+2\kappa}a^2}{\ell^4}\Big)$ and Cauchy-Schwarz

$$\begin{aligned} &\frac{1}{N^2} \sum_{\substack{p_1,p_2\in P_H \\ u_1,u_2,v_1,v_2\in P_L}} \eta_{p_1} N^{3-2\kappa} \lambda_\ell (\hat{\chi}_\ell * \hat{f}_N)(p_2) \,\mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1,u_2+p_2} \delta_{v_1-p_1,v_2-p_2} \\ &\qquad \leq CN^\kappa \|\eta\|_{L^2(P_H)} \|\hat{\chi}_\ell * \hat{f}_N\|_{L^2(P_H)} \\ &\qquad \leq CN^{-1/2+\delta_H/2+2\kappa} \|\mathcal{F}^{-1}(\chi_\ell \cdot f_N)\|_{L^2(\Lambda^*)} \\ &\qquad \leq CN^{-1/2+\delta_H/2+2\kappa}. \end{aligned}$$

We used the Convolution Theorem in the second inequality, $0 \leq f_N \leq 1$ and that the Fourier transform is an unitary map on $L^2(\Lambda)$ in the third inequality.
The second term on the r.h.s. of (4.5.13) cancels partially with terms from $\mathrm{Tr}\,[\eta^* V \eta \tilde{\Gamma}_0]$ and will be estimated later in subsection 4.5.3.
The bound for the term 4.5.11 can be obtained as follows. Applying Wick's theorem on $\mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0]$ and the fact that $\tilde{\Gamma}_0$ does not contain momentum modes in $P_L^c$ implies $u_2, v_2 \in P_L$ for nonzero contributions. Because $(p_2, u_2, v_2) \in (P_H \times P_L \times P_L)^c$ we therefore have $p_2 \in P_H^c$. Thus we can write

$$
\begin{aligned}
&\frac{1}{2N^{2-\kappa}} \sum_{\substack{p_1 \in P_H, u_1, v_1 \in P_L \\ (p_2,u_2,v_2) \in (P_H \times P_L \times P_L)^c}} \eta_{p_1} \hat{V}(p_2/N^{1-\kappa}) \,\mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1, u_2+p_2} \delta_{v_1-p_1, v_2-p_2} \\
&\quad \leq \frac{1}{2N^{2-\kappa}} \sum_{\substack{p_1 \in P_H, p_2 \in P_H^c \\ u_1, u_2, v_1, v_2 \in P_L}} \left| \eta_{p_1} \hat{V}(p_2/N^{1-\kappa}) \right| \mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \delta_{u_1+p_1, u_2+p_2} \delta_{v_1-p_1, v_2-p_2} \\
&\quad \leq \frac{1}{2N^{2-\kappa}} \sum_{u_1, u_2, v_1, v_2 \in P_L} \mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0] \left( \sum_{p \in P_H} \left| \eta_p \hat{V}((p + u_1 - u_2)/N^{1-\kappa}) \chi\left\{ \left| p + u_1 - u_2 \right| < N^{1-\delta_H} \right\} \right| \right) \\
&\quad \leq C N^{\kappa} \int_{\{N^{1-\delta_H} \leq |p| \leq N^{1-\delta_H} + 2N^{1/3+\delta_L}\}} \frac{N^{\kappa}}{p^2} dp \\
&\quad \leq C N^{1/3+\delta_L+2\kappa}.
\end{aligned}
$$

Here we used $\|\hat{V}\|_\infty < \infty$, Lemma 4.3.7, and Lemma 2.5.1.

### 4.5.3 Bound for the Interaction Energy Remainder

This subsection is devoted to the estimation of the third term on the r.h.s of (4.5.3) and the remaining term (4.5.13) from the previous subsection. The third term in (4.5.3) is given by

$$
\begin{aligned}
&\mathrm{Tr}\,[\eta^* \mathcal{V}_N \eta \Gamma_0] \\
&\quad = \frac{1}{8N^{3-\kappa}} \sum_{\substack{p_1, p_3 \in P_H \\ u_1, u_3, v_1, v_3 \in P_L \\ p_2, u_2, v_2 \in \Lambda^*}} \eta_{p_1} \hat{V}(p_2/N^{1-\kappa}) \eta_{p_3} \,\mathrm{Tr}\,[a^*_{u_1} a^*_{v_1} a_{u_1+p_1} a_{v_1-p_1} a^*_{u_2+p_2} a^*_{v_2-p_2} a_{u_2} a_{v_2} a^*_{u_3+p_3} a^*_{v_3-p_3} a_{u_3} a_{v_3} \tilde{\Gamma}_0].
\end{aligned}
\tag{4.5.14}
$$

As we have $u + p \notin P_L$ for $u \in P_L$, $p \in P_H$ for $N$ large enough, we notice that due to the energy cutoff in $\tilde{\Gamma}_0$ only commutators containing $a_{u_1+p_1}, a_{v_1-p_1}, a^*_{u_3+p_3}, a^*_{v_3-p_3}$ give non-zero contributions. We distinguish three different cases:

Let us first assume that they are contracted amongst themselves. It is enough to consider one of the two possible contractions as they give the same result. To see this, we use the to radial symmetry of $\eta_p$ and $P_H$. Using Lemma 4.3.7, Cauchy-Schwarz, $\|\hat{V}\|_\infty < C$, and Lemma 4.3.2, these terms can be

bounded in the following way

$$\frac{1}{8N^{3-\kappa}} \sum_{\substack{p_1,p_3\in P_H\\ u_1,u_3,v_1,v_3\in P_L\\ p_2,u_2,v_2\in\Lambda^*}} \eta_{p_1}\hat{V}(p_2/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{u_2}a_{v_2}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\delta_{u_1+p_1,u_3+p_3}\delta_{v_1-p_1,v_3-p_3}$$
$$\leq CN^{1+\kappa}\|\eta(\cdot)\|^2_{L^2(P_H)} \leq CN^{\delta_H+3\kappa}.$$

Next, we consider the case when they are partially contracted among themselves and partially with the operators $a^*_{u_2+p_2}, a^*_{v_2-p_2}, a_{u_2}, a_{v_2}$. Due to the radial symmetries of $P_H$ and $\eta_p$ we can assume that w.l.o.g $a_{v_1-p_1}$ is contracted with $a^*_{v_2-p_2}$, $a_{u_1+p_1}$ with $a^*_{u_3+p_3}$ and $a^*_{v_3-p_3}$ either with $a_{u_2}$ or $a_{v_2}$. We show the latter case, i.e. $a^*_{v_3-p_3}$ is contracted with $a_{v_2}$. The other case follows equivalently. We write

$$\frac{C}{N^{3-\kappa}} \sum_{\substack{p_1,p_3\in P_H\\ u_1,u_3,v_1,v_3\in P_L\\ p_2,u_2,v_2\in\Lambda^*}} \eta_{p_1}\hat{V}(p_2/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a^*_{u_2+p_2}a_{u_2}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\delta_{v_1-p_1,v_2-p_2}\delta_{u_1+p_1,u_3+p_3}\delta_{v_3-p_3,v_2}$$
$$\leq CN^{\kappa}\|\eta(\cdot)\|^2_{L^2(P_H)} \leq CN^{-1+\delta_H+3\kappa}.$$

Here we used again Lemma (4.3.2), Cauchy-Schwarz and $\|\hat{V}\|_\infty < C$.

The case when $a_{v_1-p_1}, a_{u_1+p_1}$ are contracted with $a^*_{v_2-p_2}, a^*_{u_2+p_2}$ and $a_{v_2}, a_{u_2}$ with $a^*_{v_3-p_3}, a^*_{u_3+p_3}$ is more complicated. In particular, we have to use a cancellation with the term in (4.5.13) obtained from $\mathrm{Tr}[\eta^*(\mathcal{K}+V)\tilde{\Gamma}_0]$. The contractions result in the term

$$\begin{aligned}
&\frac{1}{8N^{3-\kappa}} \sum_{\substack{p_1,p_3\in P_H\\ u_1,u_3,v_1,v_3\in P_L\\ p_2,u_2,v_2\in\Lambda^*}} \eta_{p_1}\hat{V}(p_2/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\\
&\qquad\cdot\Big(\delta_{v_1-p_1,v_2-p_2}\delta_{u_1+p_1,u_2+p_2}+\delta_{v_1-p_1,u_2+p_2}\delta_{u_1+p_1,v_2-p_2}\Big)\Big(\delta_{u_2,u_3+p_3}\delta_{v_2,v_3-p_3}+\delta_{u_2,v_3-p_3}\delta_{v_2,u_3+p_3}\Big)\\
&=\frac{1}{2N^{3-\kappa}} \sum_{\substack{p_1,p_3\in P_H\\ u_1,u_3,v_1,v_3\in P_L\\ p_2,u_2,v_2\in\Lambda^*}} \eta_{p_1}\hat{V}(p_2/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\delta_{v_1-p_1,v_2-p_2}\delta_{u_1+p_1,u_2+p_2}\delta_{u_2,u_3+p_3}\delta_{v_2,v_3-p_3}\\
&=\frac{1}{2N^{3-\kappa}} \sum_{\substack{p_1,p_3\in P_H\\ u_1,u_3,v_1,v_3\in P_L}} \eta_{p_1}\hat{V}((p_1-p_3+v_3-v_1)/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]. \qquad (4.5.15)
\end{aligned}$$

In the first equality we used radial symmetry of the set $P_H$ and of the functions $\eta_p$ and $\hat{V}$. In the second equality we used that the delta functions imply $p_2 = p_1 + v_2 - v_1 = p_1 - p_3 + v_3 - v_1$ and $u_1 + p_1 = u_2 + p_2 = u_3 + p_1 + v_3 - v_1$ which implies $u_1 + v_1 = u_3 + v_3$. The latter condition is automatically fullfilled because of the factor $\mathrm{Tr}[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\Gamma_0]$.

The term (4.5.13) can be rewritten in a similar fashion

$$
\begin{aligned}
&-\frac{1}{N^2}\sum_{\substack{p_1,p_2\in P_H\\ u_1,u_2,v_1,v_2\in P_L}}\eta_{p_1}\left(\frac{1}{2N}\sum_{q\in\Lambda^*}N^\kappa\hat{V}((p_2-q)/N^{1-\kappa})\eta_q\right)\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0]\delta_{u_1+p_1,u_2+p_2}\delta_{v_1-p_1,v_2-p_2}\\
&\quad=-\frac{1}{2N^{3-\kappa}}\sum_{\substack{p_1\in P_H,p_3\in\Lambda^*\\ u_1,u_3,v_1,v_3\in P_L}}\eta_{p_1}\hat{V}((p_1-p_3+v_3-v_1)/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\,\chi\Big\{(p_1+v_3-v_1)\in P_H\Big\}.
\end{aligned}
\tag{4.5.16}
$$

Here we renamed $q\to p_3$, $u_2\to u_3$, $v_2\to v_3$, and $p_2$ is expressed as $p_2=p_1+v_3-v_1$.
Adding (4.5.16) to (4.5.15) gives

$$
\begin{aligned}
&\frac{1}{2N^{3-\kappa}}\sum_{\substack{p_1,p_3\in P_H\\ u_1,u_3,v_1,v_3\in P_L}}\eta_{p_1}\hat{V}((p_1-p_3+v_3-v_1)/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\\
&-\frac{1}{2N^{3-\kappa}}\sum_{\substack{p_1\in P_H,p_3\in\Lambda^*\\ u_1,u_3,v_1,v_3\in P_L}}\eta_{p_1}\hat{V}((p_1-p_3+v_3-v_1)/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\chi\Big\{(p_1+v_3-v_1)\in P_H\Big\}\\
&\quad=\frac{1}{2N^{3-\kappa}}\sum_{\substack{p_1\in P_H,p_3\in\Lambda^*\\ u_1,u_3,v_1,v_3\in P_L}}\eta_{p_1}\hat{V}((p_1-p_3+v_3-v_1)/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\chi\Big\{(p_1+v_3-v_1)\in P_H^c\Big\}\\
&\qquad-\frac{1}{2N^{3-\kappa}}\sum_{\substack{p_1\in P_H,p_3\in P_H^c\\ u_1,u_3,v_1,v_3\in P_L}}\eta_{p_1}\hat{V}((p_1-p_3+v_3-v_1)/N^{1-\kappa})\eta_{p_3}\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\\
&\quad:=\mathcal{R}_3+\mathcal{R}_4.
\end{aligned}
$$

To give a bound for the term $\mathcal{R}_3$ we need the following estimate, which can be found in [2] equation (3.12):

$$
\sup_{p\in\Lambda^*}\Big|\hat{V}(\,\cdot\,/N^{1-\kappa})*\eta(p)\Big|\le C(N+N^\kappa).
\tag{4.5.17}
$$

Using the bound (4.3.7), the estimate (4.5.17) and Lemma 2.5.1 we can write for $\mathcal{R}_3$

$$
\begin{aligned}
\mathcal{R}_3&=\frac{1}{2N^{3-\kappa}}\sum_{\substack{p_1\in P_H\\ u_1,u_3,v_1,v_3\in P_L}}\eta_{p_1}\chi\Big\{(p_1+v_3-v_1)\in P_H^c\Big\}[\hat{V}(\,\cdot\,/N^{1-\kappa})*\eta](p_1+v_3-v_1)\,\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\\
&\le\frac{1}{2N^{3-\kappa}}\sup_{p\in\Lambda^*}\Big|\hat{V}(\,\cdot\,/N^{1-\kappa})*\eta(p)\Big|\left(\sum_{p_1\in P_H}|\eta_{p_1}|\chi\Big\{|p_1|\le N^{1-\delta_H}+2N^{1/3+\delta_L}\Big\}\right)\\
&\quad\cdot\left(\sum_{u_1,u_3,v_1,v_3\in P_L}\mathrm{Tr}\,[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0]\right)\\
&\le CN^\kappa\int_{\{N^{1-\delta_H}\le|p|\le N^{1-\delta_H}+2N^{1/3+\delta_L}\}}\frac{N^\kappa}{p^2}dp\\
&\le CN^{1/3+\delta_L+2\kappa}.
\end{aligned}
$$

Applying Hölder with $3/2 < p \leq 2$, $1/p + 1/q = 1$ on the sum over $P_H$ in $\mathcal{R}_4$ and completing the sum to $\left\|\hat{V}(\cdot/N^{1-\kappa})\right\|_{L^q(\Lambda^*)}$, gives

$$\mathcal{R}_4 \leq \frac{C}{N^{3-\kappa}} \sum_{\substack{r\in P_H^c \\ u_1,u_3,v_1,v_3\in P_L}} \|\eta\|_{L^p(P_H)} \left\|\hat{V}(\,\cdot\,/N^{1-\kappa})\right\|_{L^q(\Lambda^*)} |\eta_r| \operatorname{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_3}a_{v_3}\tilde{\Gamma}_0\right]. \tag{4.5.18}$$

Applying Lemma 2.5.1 and the bound (4.3.6) we obtain

$$\|\eta\|_{L^p(P_H)} \leq CN^{\kappa}\left(\int_{N^{1-\delta_H}-\sqrt{12}\pi}^{\infty} s^{2-2p}ds\right)^{1/p} \leq CN^{\kappa+(1-\delta_H)(3-2p)/p}. \tag{4.5.19}$$

Applying the Hausdorff-Young inequality for $2 \leq q < 3$ and using $V \in L^p(\mathbb{R}^3)$ for $3/2 < p \leq 2$ we get

$$\left\|\hat{V}(\,\cdot\,/N^{1-\kappa})\right\|_{L^q(\Lambda^*)} \leq N^{3(1-\kappa)}\left\|V(\,\cdot\,N^{1-\kappa})\right\|_{L^p(\Lambda)} \leq C\left\|V\right\|_{L^p(\Lambda)}N^{3(1-\kappa)-3(1-\kappa)/p} \leq CN^{3(1-\kappa)/q}. \tag{4.5.20}$$

An application of Lemma 2.5.1 and the bound (4.3.6) yield

$$|\eta_0| + \sum_{r\in P_H^c\setminus\{0\}} |\eta_r| \leq CN^{\kappa} + CN^{1-\delta_H+\kappa} \leq CN^{1-\delta_H+\kappa}. \tag{4.5.21}$$

Applying the Lemma 4.3.7, the bounds (4.5.19), (4.5.20) and (4.5.21) to (4.5.18) we obtain

$$\begin{aligned}\mathcal{R}_4 &\leq CN^{\kappa-3}N^{\kappa+(1-\delta_H)(3-2p)/p}N^{3(1-\kappa)/q}N^{1-\delta_H+\kappa}N^2 \\ &= CN^{3\kappa/p}N^{1+\delta_H-3\delta_H/p}.\end{aligned} \tag{4.5.22}$$

Putting the above considerations together, we get the following bound for the second and third term in (4.5.3)

$$\operatorname{Tr}\left[\eta^*(\mathcal{V}_N+\mathcal{K})\tilde{\Gamma}_0\right] + \operatorname{Tr}\left[\eta^*\mathcal{V}_N\eta\tilde{\Gamma}_0\right] \leq CN^{-1/2+\delta_H/2+2\kappa} + CN^{1/3+\delta_L+2\kappa} + CN^{\delta_H+3\kappa} + CN^{1+\delta_H-3\delta_H/p+3\kappa/p}, \tag{4.5.23}$$

where $3/2 < p \leq 2$.

### 4.5.4 Bound for the Kinetic Energy Remainder

In this subsection we derive a bound for the fourth term on the r.h.s of equation (4.5.3). We write

$$\begin{aligned}\operatorname{Tr}\left[(\mathcal{K}+(1+\eta^*)\mathcal{K}_L)\tilde{\Gamma}_0\right] &= \frac{1}{N}\sum_{p\in P_H,u,v\in P_L} \eta_p p^2 \operatorname{Tr}\left[a^*_{u+p}a^*_{v-p}a_ua_v\tilde{\Gamma}_0\right] \\ &\quad + \frac{1}{N}\sum_{p\in P_H,u,v\in P_L} \eta_p p\cdot(u-v)\operatorname{Tr}\left[a^*_{u+p}a^*_{v-p}a_ua_v\tilde{\Gamma}_0\right] \\ &\quad + \frac{1}{2N^2}\sum_{\substack{p_1,p_2\in P_H \\ u_1,v_1,u_2,v_2\in P_L}} \eta_{p_1}\eta_{p_2}p_2\cdot(u_2-v_2)\operatorname{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right] \\ &= \frac{1}{2N^2}\sum_{\substack{p_1,p_2\in P_H \\ u_1,v_1,u_2,v_2\in P_L}} \eta_{p_1}\eta_{p_2}p_2\cdot(u_2-v_2)\operatorname{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_2}a_{v_2}\tilde{\Gamma}_0\right] \\ &\qquad \cdot\left(\delta_{u_1+p_1,u_2+p_2}\delta_{v_1-p_1,v_2-p_2} + \delta_{u_1+p_1,v_2-p_2}\delta_{v_1-p_1,u_2+p_2}\right)\end{aligned} \tag{4.5.24}$$

In the second equality we used that the one-particle density matrix of $\tilde{\Gamma}_0$ is diagonal in Fourier space and that $\delta_{u+p,u} = \delta_{u+p,v} = 0$ for $p \in P_H, u, v \in P_L$. Thus the first two terms vanish. Moreover, due to the momentum cutoff in $\tilde{\Gamma}_0$ we only have to consider commutators of $a_{u_1+p_1}, a_{v_1-p_1}$ with $a^*_{u_2+p_2}, a^*_{v_2-p_2}$ in the third term.

To continue we first need some intermediate results. We choose two constants $q, r$ s.t. $q > 1 - \delta_H$ and $r > 1$. An application of Lemma 2.5.1 and the bound (4.3.6) implies for $u \in 2P_L$ and $N$ large enough

$$\begin{aligned}\sum_{\substack{p_2\in P_H\\ |p_2|\leq rN^q}} |\eta_{u+p_2}||\eta_{p_2}||p_2| &\leq CN^{2\kappa} \sum_{\substack{p_2\in P_H\\ |p_2|\leq rN^q}} \frac{1}{|p_2|(|p_2| - 2N^{1/3+\delta_L})^2} \leq CN^{2\kappa} \int_{N^{1-\delta_H}}^{rN^q} \frac{p}{(p - 2N^{1/3+\delta_L})^2} dp \\ &\leq CN^{2\kappa} \int_{N^{1-\delta_H}-2N^{1/3+\delta_L}}^{rN^q-2N^{1/3+\delta_L}} \frac{2}{p} dp \leq CN^{2\kappa} \ln\left(rN^q - 2N^{1/3+\delta_L}\right) \\ &\leq C_{q,r} N^{2\kappa} \ln(N)\,. \end{aligned} \tag{4.5.25}$$

Define the set $P_{q,r} := \{p \in \Lambda^* || p| > rN^q\}$. Using the estimate (4.3.6) and Lemma 2.5.1 we obtain the bound

$$\|\eta_p\|_{L^2(P_{q,r})} \leq C_r N^{\kappa - q/2}. \tag{4.5.26}$$

An application of Plancherel and Lemma 2.5.1 yields

$$\begin{aligned}\|p\eta_p\|_{L^2(P_{q,r})} &\leq \left(\int \left|\nabla(-Nw_l(N^{1-\kappa}x))\right|^2 dx\right)^{1/2} = \left(N^{1+\kappa} \int \left|\nabla w_l(x)\right|^2 dx\right)^{1/2} \\ &\leq N^{1/2+\kappa/2} \left(\int \frac{C}{(|x|^2+1)^2} dx\right)^{1/2} \leq CN^{1/2+\kappa/2}. \end{aligned} \tag{4.5.27}$$

Moreover, we have the following bound

$$\begin{aligned}\sum_{u_1,v_1,u_2,v_2\in P_L} \left|u_2 - v_2\right| \operatorname{Tr}\left[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0\right] &\leq 2 \sum_{u_1,v_1,u_2,v_2\in P_L} |u_2| \operatorname{Tr}\left[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0\right] \\ &\leq 4 \sum_{u,v\in P_L} |u|\hat{\gamma}_0(u)\hat{\gamma}_0(v) \leq 4N \sum_{u\in P_L} |u|\hat{\gamma}_0(u) \leq CN^{1+1/3}. \end{aligned} \tag{4.5.28}$$

Here we used a Riemann sum approximation in the last inequality. Using the estimates (4.5.25), (4.5.26), (4.5.27) and (4.5.28) we can write for the r.h.s of (4.5.24)

$$\begin{aligned}&\frac{1}{2N^2} \sum_{\substack{p_1,p_2\in P_H\\ u_1,v_1,u_2,v_2\in P_L}} \eta_{p_1}\eta_{p_2} p_2 \cdot (u_2 - v_2) \operatorname{Tr}\left[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0\right] \left(\delta_{u_1+p_1,u_2+p_2}\delta_{v_1-p_1,v_2-p_2} + \delta_{u_1+p_1,v_2-p_2}\delta_{v_1-p_1,u_2+p_2}\right) \\ &\quad\leq \frac{C}{N^2} \sum_{u_1,v_1,u_2,v_2\in P_L} |u_2 - v_2| \operatorname{Tr}\left[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0\right] \sup_{u\in 2P_L} \left(\sum_{p_2\in P_H} |\eta_{u+p_2}||\eta_{p_2}||p_2| \chi\left(u + p_2 \in P_H\right)\right) \\ &\quad\leq \frac{C}{N^2} \sum_{u_1,v_1,u_2,v_2\in P_L} |u_2 - v_2| \operatorname{Tr}\left[a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \tilde{\Gamma}_0\right] \\ &\qquad\qquad \cdot \sup_{u\in P_L+P_L} \left(\sum_{p_2\in P_H\setminus P_{q,r}} |\eta_{u+p_2}||\eta_{p_2}||p_2| + \sum_{p_2\in P_{q,r}} |\eta_{u+p_2}||\eta_{p_2}||p_2| \chi\left(u + p_2 \in P_H\right)\right) \\ &\quad\leq N^{1/3} \left(C_{q,r} N^{2\kappa} \ln(N) + \|\eta_p\|_{L^2(P_{q,r})} \|p\eta_p\|_{L^2(P_{q,r})}\right) \\ &\quad\leq CN^{1/3+2\kappa} \ln(N). \end{aligned}$$

In the third inequality we applied Cauchy-Schwarz. To obtain the fourth inequality we chose $q = 1-\kappa$. We obtain the following bound for the fourth term in (4.5.3)

$$\mathrm{Tr}[(\mathcal{K} + (1+\eta^*)\mathcal{K}_L)\tilde{\Gamma}_0] \leq CN^{1/3+2\kappa}\ln(N). \tag{4.5.29}$$

## 4.6 Estimation of the Entropy

To give a bound for the entropy we will apply Lemma 4.3.8 for the projections $P_\alpha = |\phi_\alpha\rangle\langle\phi_\alpha| = \frac{|(1+\eta)\psi_\alpha\rangle\langle(1+\eta)\psi_\alpha|}{\langle(1+\eta)\psi_\alpha|(1+\eta)\psi_\alpha\rangle}$ and the state $\tilde{\Gamma}_0$. This gives us

$$S(\Gamma) \geq S(\tilde{\Gamma}_0) - \ln\left(\sum_{\alpha=1}^{\infty}\mathrm{Tr}\left[P_\alpha\Gamma\right]\right). \tag{4.6.1}$$

To estimate the sum in the logarithm we need the following inequality where $\delta > 0$

$$(x+y)^2 = x^2 + y^2 + 2x\delta^{1/2}\frac{y}{\delta^{1/2}} \leq x^2\left(1+\delta\right) + y^2\left(1+\delta^{-1}\right). \tag{4.6.2}$$

We estimate

$$\begin{aligned}
\sum_{\alpha=1}^{\infty}\mathrm{Tr}[P_\alpha\Gamma] &= \sum_{\alpha,\beta=1}^{\infty}\lambda_\beta\left|\langle\phi_\alpha|\phi_\beta\rangle\right|^2 = \sum_{\alpha,\beta=1}^{\infty}\lambda_\beta\left|\frac{\langle(1+\eta)\psi_\alpha|(1+\eta)\psi_\beta\rangle}{||(1+\eta)\psi_\alpha||||(1+\eta)\psi_\beta||}\right|^2 \\
&\leq \sum_{\alpha,\beta=1}^{\infty}\lambda_\beta\left(\delta_{\alpha,\beta} + \left|\langle\psi_\alpha|\eta^*\eta\psi_\beta\rangle\right|\right)^2 \leq \sum_{\alpha,\beta=1}^{\infty}\lambda_\beta\left(\delta_{\alpha,\beta}\left(1+\delta\right) + \left(1+\delta^{-1}\right)|\langle\psi_\alpha|\eta^*\eta\psi_\beta\rangle|^2\right) \\
&= \left(1+\delta\right) + \left(1+\delta^{-1}\right)\sum_{\alpha=1}^{\infty}\langle\psi_\alpha|\eta^*\eta\tilde{\Gamma}_0\eta^*\eta\psi_\alpha\rangle\,.
\end{aligned} \tag{4.6.3}$$

In the first inequality we used the bound (4.4.1) and that, because of the energy cutoff in $\tilde{\Gamma}_0$, all eigenfunctions $\psi_\alpha$ do not contain high momenta. In the second inequality we applied (4.6.2). In the last line we used $\sum_{\alpha=1}^{\infty}\lambda_\alpha = 1$.
It remains to give a bound for the sum in the second term on the r.h.s of (4.6.3). Completing $\{\psi_\alpha\}_{\alpha=1}^{\infty}$ to an orthonormal basis of $\mathscr{F}_0\otimes\mathscr{F}_>$ and using that $\eta^*\eta\tilde{\Gamma}_0\eta^*\eta$ is a positive operator we find

$$\begin{aligned}
\sum_{\alpha=1}^{\infty}\langle\psi_\alpha|\eta^*\eta\tilde{\Gamma}_0\eta^*\eta\psi_\alpha\rangle &\leq \mathrm{Tr}\left[\eta^*\eta\tilde{\Gamma}_0\eta^*\eta\right] = \mathrm{Tr}\left[\eta^*\eta\eta^*\eta\tilde{\Gamma}_0\right] \\
&= \frac{1}{16N^4}\sum_{\substack{p_1,\dots,p_4\in P_H\\ u_1,v_1,\dots,u_4,v_4\in P_L}}\eta_{p_1}\dots\eta_{p_4}\,\mathrm{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{u_2}a_{v_2}\right. \\
&\qquad\qquad \left. a^*_{u_3}a^*_{v_3}a_{u_3+p_3}a_{v_3-p_3}a^*_{u_4+p_4}a^*_{v_4-p_4}a_{u_4}a_{v_4}\tilde{\Gamma}_0\right] \\
&\leq \frac{C}{N^4}\sup_{u\in 2P_L}\left(\sum_{p\in P_H}\left|\eta_p\eta_{p+u}\chi\{p+u\in P_H\}\right|\right)^2\cdot\left(\sum_{u_1,v_1,\dots,u_4,v_4\in P_L}\mathrm{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_2}a_{v_2}a^*_{u_3}a^*_{v_3}a_{u_4}a_{v_4}\tilde{\Gamma}_0\right]\right) \\
&\leq \frac{C}{N^4}||\eta||^4_{L^2(P_H)}\sum_{u_1,v_1,\dots,u_4,v_4\in P_L}\mathrm{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_2}a_{v_2}a^*_{u_3}a^*_{v_3}a_{u_4}a_{v_4}\tilde{\Gamma}_0\right] \\
&\leq CN^{-2+2\delta_H+4\kappa}.
\end{aligned} \tag{4.6.4}$$

In the first inequality we used that only commutators of $a_{u_1+p_1}, a_{v_1-p_1}$ with $a^*_{u_2+p_2}, a^*_{v_2-p_2}$ and commutators of $a_{u_3+p_3}, a_{v_3-p_3}$ with $a^*_{u_4+p_4}, a^*_{v_4-p_4}$ give non-zero contributions. Their commutators yield delta functions that contract the high momenta $p_1, p_2 \in P_H$ to one high momenta variable and the same for $p_3, p_4 \in P_H$. Applying Cauchy-Schwarz to the sum over high momenta in the second inequality gives the bound $\|\eta\|^4_{L^2(P_H)}$ for the square of this sum. In the third inequality we used Lemma 4.3.2 and Lemma 4.3.7.
Inserting (4.6.4) into (4.6.3) and choosing $\delta = N^{-1+\delta_H+2\kappa}$ yields the bound

$$\sum_{\alpha=1}^{\infty} \mathrm{Tr}\,[P_\alpha \hat{\Gamma}] \leq 1 + CN^{-1+\delta_H+2\kappa}.$$

Accordingly, we have

$$S(\Gamma) \geq S(\tilde{\Gamma}_0) - CN^{-1+\delta_H+2\kappa}. \tag{4.6.5}$$

Note that the entropy function $-x\ln(x)$ is concave. Thus we can apply Lemma 4.3.9 to extract the entropy of the distribution over coherent condensate states. Consequently we have

$$S(\tilde{\Gamma}_0) = S\left(\int_0^\infty |\sqrt{x}\rangle\langle\sqrt{x}|\, f(x)dx\right) + S\left(\Gamma_\mu^{\mathrm{ec}}\right) \geq S(f) + S(\Gamma_\mu^{\mathrm{ec}}). \tag{4.6.6}$$

For the entropy of $f$ we compute

$$S(f) = -\int_0^\infty f(x)\ln(f(x))dx = \ln(N_0) + \lambda_1 + \lambda_2(1+g(N_0)) + \ln(Z(\lambda_1,\lambda_2)). \tag{4.6.7}$$

The term $\ln(Z(\lambda_1,\lambda_2))$ can be written as

$$\begin{aligned}\ln(Z(\lambda_1,\lambda_2)) &= \ln\left(\int_0^\infty \exp\Big(-\big(\lambda_1 x + \lambda_2 x^2\big)\Big)dx\right) = \ln\left(\frac{\exp\left(\frac{\lambda_1^2}{4\lambda_2}\right)}{(2\lambda_2)^{1/2}}\int_{\frac{\lambda_1}{\sqrt{2\lambda_2}}}^\infty \exp\left(-\frac{x^2}{2}\right)dx\right)\\ &= \frac{\lambda_1^2}{4\lambda_2} - \frac{1}{2}\ln(2\lambda_2) + \ln\left(\int_{\frac{\lambda_1}{\sqrt{2\lambda_2}}}^\infty \exp\left(-\frac{x^2}{2}\right)dx\right).\end{aligned} \tag{4.6.8}$$

With the bounds (4.3.22) from Lemma 4.3.6 we get

$$\begin{aligned}S(f) &= \ln(N_0) + \lambda_1 + \lambda_2(1+g(N_0)) + \frac{\lambda_1^2}{4\lambda_2} - \frac{1}{2}\ln(2\lambda_2) + \ln\left(\int_{\frac{\lambda_1}{\sqrt{2\lambda_2}}}^\infty \exp\left(-\frac{x^2}{2}\right)dx\right)\\ &= \ln(N_0) + \frac{1}{2}\ln(g(N_0)) + 1/2 + \ln\left(\int_{-g(N_0)^{-1/2}}^\infty \exp\left(-\frac{x^2}{2}\right)dx\right) + O\Big(\exp\big(-Cg(N_0)^{-1}\big)\Big).\end{aligned} \tag{4.6.9}$$

Using that $0 < g(N_0) \ll 1$ and that the function $x \mapsto \exp(-x^2/4)$ is monotone decreasing for $x \geq 0$ we obtain

$$\varepsilon := \int_{g(N_0)^{-1/2}}^\infty \exp\left(-\frac{x^2}{2}\right)dx \leq \exp\left(-\frac{g(N_0)^{-1}}{4}\right)\int_{g(N_0)^{-1/2}}^\infty \exp\left(-\frac{x^2}{4}\right)dx \leq C\exp\left(-\frac{g(N_0)^{-1}}{4}\right). \tag{4.6.10}$$

The concavity of the logarithm and the above bound (4.6.10) with the assumption $0 < g(N_0) \ll 1$ imply the estimate

$$\ln\left(\int_{-g(N_0)^{-1/2}}^{\infty} \exp\left(-\frac{x^2}{2}\right) dx\right) = \ln\Big(\sqrt{2\pi} - \varepsilon\Big) = \ln\left(\left(1 - \frac{\varepsilon}{\sqrt{2\pi}-1}\right)\sqrt{2\pi} + \frac{\varepsilon}{\sqrt{2\pi}-1}\right)$$
$$\geq \left(1 - \frac{\varepsilon}{\sqrt{2\pi}-1}\right)\ln\Big(\sqrt{2\pi}\Big) \geq \ln\Big(\sqrt{2\pi}\Big) - \exp\left(-\frac{g(N_0)^{-1}}{4}\right). \quad (4.6.11)$$

Thus we have

$$S(f) \geq \ln(N_0) + \frac{1}{2}\ln(g(N_0)) + \frac{1}{2} + \ln\Big(\sqrt{2\pi}\Big) + O\Big(\exp\Big(-Cg(N_0)^{-1}\Big)\Big). \quad (4.6.12)$$

Inserting (4.6.12) into (4.6.6) and combining with (4.6.5) we get

$$S(\Gamma) \geq S(\Gamma_\mu^{\mathrm{ec}}) + \ln(N_0) + \frac{1}{2}\ln(g(N_0)) + \frac{1}{2} + \ln\Big(\sqrt{2\pi}\Big) + O\Big(\exp\Big(-Cg(N_0)^{-1}\Big)\Big) + O\Big(N^{-1+\delta_H+2\kappa}\Big). \quad (4.6.13)$$

## 4.7 Thermal Free Energy of the Ideal Bose Gas

Collecting the kinetic energy of $\tilde{\Gamma}_0$ from (4.5.1) and the entropy of $\Gamma_\mu^{\mathrm{ec}}$ from (4.6.13) we write

$$\mathrm{Tr}\,[d\Gamma(-\Delta)\tilde{\Gamma}_0] - \frac{1}{\beta}S(\Gamma_\mu^{\mathrm{ec}}) = F_0^{\mathrm{ec}}(N_{\mathrm{th}}, \Lambda_L, \beta),$$

where $F_0^{\mathrm{ec}}(N_{\mathrm{th}}, \Lambda_L, \beta)$ is the free energy corresponding to the operator $H_0^{\mathrm{ec}} := \sum_{p\in P_L\setminus\{0\}} p^2 a_p^* a_p$. Using the expression on the r.h.s of equation (3.0.3) we have

$$\mathrm{Tr}\,[d\Gamma(-\Delta)\tilde{\Gamma}_0] - \frac{1}{\beta}S(\Gamma_\mu^{\mathrm{ec}}) = -\frac{1}{\beta}\ln\Big(\mathrm{Tr}\Big[\exp\big(-\beta(H_0^{\mathrm{ec}} - \mu\mathcal{N}_>)\big)\Big]\Big) + \mu N_{\mathrm{th}} = \Phi(\Gamma_\mu^{\mathrm{ec}}) + \mu N_{\mathrm{th}}, \quad (4.7.1)$$

where $\Phi(\Gamma_\mu^{\mathrm{ec}})$ is the grand potential of $\Gamma_\mu^{\mathrm{ec}}$. In the following we investigate how much the grand potential of $\Gamma_\mu^{\mathrm{ec}}$ differs from the grand potential of $\Gamma_{\mu_0}^0$. Using a similar calculation as in (2.4.2) we write

$$\begin{aligned}
\Phi(\Gamma_\mu^{\mathrm{ec}}) - \Phi(\Gamma_{\mu_0}^0) &= -\frac{1}{\beta}\ln\Big(\mathrm{Tr}\,[Z_\mu^{\mathrm{ec}}]\Big) + \frac{1}{\beta}\ln\Big(\mathrm{Tr}\,[Z_{\mu_0}^0]\Big) \\
&= \frac{1}{\beta}\ln\left[\prod_{p\in P_L\setminus\{0\}}\Big(1 - \exp\big(-\beta(p^2-\mu)\big)\Big)\right] - \frac{1}{\beta}\ln\left[\prod_{p\in\Lambda_+^*}\Big(1 - \exp\big(-\beta(p^2-\mu_0)\big)\Big)\right] \\
&= \frac{1}{\beta}\sum_{p\in P_L\setminus\{0\}}\Big[\ln\Big(1 - \exp\big(-\beta(p^2-\mu)\big)\Big) - \ln\Big(1 - \exp\big(-\beta(p^2-\mu_0)\big)\Big)\Big] \\
&\quad - \frac{1}{\beta}\sum_{p\in P_L^c}\ln\Big(1 - \exp\big(-\beta(p^2-\mu_0)\big)\Big) \quad (4.7.2)
\end{aligned}$$

The first term on the r.h.s of (4.7.2) is negative because the function $f_p(x) := \ln(1-\exp(-\beta(p^2-x)))$ is monotone decreasing for $x < p^2$ and due to Lemma 4.3.5 we have $\mu_0 < \mu$ and moreover $\mu < 4\pi^2 \leq p^2$ for any $p \in P_L \setminus \{0\}$. For the summands in the second term of (4.7.2) we use the estimate

$$-\ln(1-x) = \sum_{n=1}^{\infty} \frac{x^n}{n} \leq x \sum_{n=0}^{\infty} x^n = \frac{x}{1-x} \leq 2x, \quad \text{for } x \in [0, 1/2].$$

This estimate can be applied because for $N$ large enough we have $\exp(-\beta(p^2-\mu_0)) < 1/2$ for any $p \in P_L^c$. Consequently we find a constant $c > 0$ such that we have

$$\Phi(\Gamma_\mu^{\mathrm{ec}}) - \Phi(\Gamma_{\mu_0}^0) \leq \frac{2}{\beta} \sum_{p \in P_L^c} \exp(-\beta(p^2-\mu_0)) \leq C \exp(-cN^{2\delta_L}). \tag{4.7.3}$$

In the last inequality we used an integral approximation with the same arguments as in the proof of Lemma 4.3.3.
Combining (4.7.1), (4.7.3) and an application of Lemma 4.3.5 yields

$$\begin{aligned}\mathrm{Tr}\,[d\Gamma(-\Delta)\tilde{\Gamma}_0] - \frac{1}{\beta} S(\Gamma_\mu^{\mathrm{ec}}) = \Phi(\Gamma_\mu^{\mathrm{ec}}) + \mu N_{\mathrm{th}} &= \Phi(\Gamma_{\mu_0}^0) + \mu_0 N_{\mathrm{th}} + \Big(\Phi(\Gamma_\mu^{\mathrm{ec}}) - \Phi(\Gamma_{\mu_0}^0)\Big) + (\mu-\mu_0)N_{\mathrm{th}} \\ &\leq F_0^{\mathrm{th}}(N_{\mathrm{th}}, \Lambda_L, \beta) + O\left(\exp(-CN^{2\delta_L})\right).\end{aligned} \tag{4.7.4}$$

Here $F_0^{\mathrm{th}}(N_{\mathrm{th}}, \Lambda_L, \beta)$ denotes the free energy of the thermal cloud of the ideal Bose gas.

## 4.8 Combining the derived Bounds

Combining (4.5.9), (4.5.23), (4.5.29) we obtain the following upper bound for the correlation energy

$$\begin{aligned}\mathrm{Tr}\left[(1+\eta^*)\Big([H_0,\eta] + \mathcal{V}_N(1+\eta)\Big)\tilde{\Gamma}_0\right] \leq \frac{1}{N^{1-\kappa}} 4\pi a\Big(N_0^2(1+g(N_0)) + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\Big) \\ + O\Big(N^{1-\delta_H+2\kappa} + N^{1/3+\delta_L+2\kappa} + N^{\delta_H+3\kappa} + N^{1+\delta_H-3\delta_H/p+3\kappa/p}\Big).\end{aligned} \tag{4.8.1}$$

Here we have $3/2 < p \leq 2$, $\delta_H, \delta_L > 0$, with $\delta_H + \delta_L < 2/3$. In the derivation of the energy and entropy the only other terms containing $\delta_H, \delta_L$ are of order $\exp(-CN^{2\delta_L})$ (see equation (4.7.4)) or $N^{-1+\delta_H+2\kappa}$ (see equation (4.6.13)) which are of smaller order than the errors in (4.8.1). The deviation of $N_0$ from $\tilde{N}_0$ is at most in order of $N^{\delta_H+2\kappa}$ and therefore contained in the bound (4.8.1). Thus we can already optimize the bound (4.8.1) over the parameters $p, \delta_L, \delta_H$.
As discussed in chapter 4.2 we set $\kappa = 0$. Let $0 < \varepsilon \leq 1/6$, then we set $p = 3/(2-2\varepsilon)$, $\delta_H = 1/2$, $0 < \delta_L < 1/6$ which yields the bound

$$\mathrm{Tr}\left[(1+\eta^*)\Big([H_0,\eta] + \mathcal{V}_N(1+\eta)\Big)\tilde{\Gamma}_0\right] \leq \frac{1}{N} 4\pi a\Big(N_0^2(1+g(N_0)) + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\Big) + O\left(N^{1/2+\varepsilon}\right). \tag{4.8.2}$$

Combining the estimates (4.5.1), (4.6.13), (4.7.4), (4.8.2) and multiplying the scaling factor $L^{-2}$ to the energy contributions gives the bound

$$\begin{aligned}\mathrm{Tr}\,[H_N\Gamma] - \frac{1}{\beta}S(\Gamma) \leq F_0^{\mathrm{th}}(N,\Lambda_L,\beta) + 4\pi a_N L^{-3}\Big(N_0^2 + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\Big)\\ + 4\pi a_N L^{-3}N_0^2 g(N_0) - \frac{1}{2\beta}\ln\Big(2\pi e N_0^2 g(N_0)\Big)\\ + \beta^{-1}O\Big(\exp\Big(-Cg(N_0)^{-1}\Big)\Big) + O\left(\frac{N^{1/2+\varepsilon}}{L^2}\right).\end{aligned} \tag{4.8.3}$$

Neglecting the error term $\beta^{-1}O(\exp(-Cg(N_0)^{-1}))$, $g(N_0)$ attains its minimum at $g(N_0) = \left(\beta 8\pi a_N L^{-3}N_0^2\right)^{-1}$. Note that the expression for $g(N_0)$ is only suitable for our proof if we have $\beta \geq \beta_c(1+\delta)$ with $\delta > 0$. We can see this using equation (2.4.12) and writing

$$\begin{aligned}g(N_0) = \left(\beta 8\pi a_N L^{-3}N_0^2\right)^{-1} = O\left(N_0^{-1/3}\left(\frac{N_0}{N}\right)^{-5/3}\right) = O\left(N^{-1/3}\left[1-\left(\frac{\beta_c}{\beta}\right)^{3/2}\right]^{-2}\right)\\ \leq O\left(N^{-1/3}\left[1-\frac{1}{(1+\delta)^{3/2}}\right]^{-2}\right) \leq O\left(N^{-1/3}\delta^{-2}\right).\end{aligned} \tag{4.8.4}$$

Here we used that the function $f(x) = (1-x^{-3/2})$ is concave which implies $f(1+\delta) \geq (1-\alpha)f(1) + \alpha f(c) \geq C\delta$ where $c > 1+\delta$, $\alpha = \delta/(c-1)$. Thus to fulfill the condition $0 < g(N_0) \ll 1$ we have to assume $\delta \geq N^{-1/6+\varepsilon_1}$ for some $\varepsilon_1 > 0$. For $N$ large enough this certainly holds. For the rest of the proof, we assume $\beta > \beta_c(1+\delta)$ with $\delta \geq N^{-1/6+\varepsilon_1}$ for $\varepsilon_1 > 0$.
Inserting the optimized $g(N_0)$ into the bound (4.8.5) we get

$$\begin{aligned}\mathrm{Tr}\,[H_N\Gamma] - \frac{1}{\beta}S(\Gamma) \leq F_0^{\mathrm{th}}(N,\Lambda_L,\beta) + 4\pi a_N L^{-3}\Big(N_0^2 + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\Big)\\ + \frac{1}{2\beta}\ln\Big(\beta 4a_N L^{-3}\Big) + O\left(\frac{N^{1/2+\varepsilon}}{L^2}\right).\end{aligned} \tag{4.8.5}$$

The estimate (4.2.17) and the choices $\delta_H = 1/2$, $\kappa = 0$ give $|\tilde{N}_0 - N_0| \leq CN^{1/2}$. Thus we have

$$\begin{aligned}4\pi a_N L^{-3}\Big(N_0^2 + 4N_0N_{\mathrm{th}} + 2N_{\mathrm{th}}^2\Big) \leq 4\pi a_N L^{-3}\Big(2N^2 - \tilde{N}_0^2 + CN^{3/2}\Big)\\ = 4\pi a_N L^3\Big(2\varrho^2 - \varrho_0^2(N,\Lambda_L,\beta)\Big) + O(L^{-2}N^{1/2}),\end{aligned} \tag{4.8.6}$$

where $\varrho_0(N,\Lambda_L,\beta) = \tilde{N}_0L^{-3}$ is the expected condensate density of the ideal Bose gas with particle number expectation $N$. Together with the Gibbs variational principle we obtain the desired final bound

$$\begin{aligned}F(N,\Lambda_L,\beta) \leq \mathrm{Tr}\,[H_N\Gamma] - \frac{1}{\beta}S(\Gamma)\\ \leq F_0^{\mathrm{th}}(N_{\mathrm{th}},\Lambda_L,\beta) + 4\pi a_N L^3\Big(2\varrho^2 - \varrho_0^2(N,\Lambda_L,\beta)\Big) + \frac{1}{2\beta}\ln\Big(\beta 4a_N L^{-3}\Big) + O\left(\frac{N^{1/2+\varepsilon}}{L^2}\right).\end{aligned} \tag{4.8.7}$$

# Bibliography


[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, E.A. Cornell, *Observation of bose-einstein condensation in a dilute atomic vapor*, Science **269**, 198 (1995)

[2] G. Basti, S. Cenatiempo, B. Schlein, *A new second-order upper bound for the ground state energy of dilute Bose gases*, Forum of Mathematics, Sigma **9**, E74 (2021)

[3] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein, *Bogoliubov Theory in the Gross-Pitaevskii Limit*, Acta Math. **222**, 219 (2019)

[4] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein, *Optimal rate for Bose-Einstein condensation in the Gross-Pitaevskii regime*, Commun. Math. Phys. **376**, 1311 (2020)

[5] N.N. Bogoliubov, *On the theory of superfluidity* Izv. Akad. Nauk USSR **11**, 77 (1947). Eng. Trans. J. Phys. (USSR), **11**, 23 (1947)

[6] N.N. Bogoliubov, *Energy levels of the imperfect Bose-Einstein gas* Bull. Moscow State Univ. **7**, 43 (1947)

[7] M. Combescure, D. Robert, *Coherent States and Applications in Mathematical Physics*, Springer, Dordrecht (2012)

[8] A. Deuchert, P. T. Nam, M. Napiorkowski *Free energy of the weakly interacting homogeneous Bose gas*, unpublished

[9] A. Deuchert, R. Seiringer, *Gross-Pitaevskii Limit of a Homogeneous Bose Gas at Positive Temperature*, Arch. Rational Mech. Anal. **236**(3), 1217 (2020)

[10] A. Deuchert, R. Seiringer, J. Yngvason, *Bose-Einstein Condensation for a Dilute Trapped Gas at Positive Temperature*, Commun. Math. Phys. **368**, 723 (2019)

[11] L. Erdős, B. Schlein, H.-T. Yau. *Derivation of the Gross-Pitaevskii hierarchy for the dynamics of Bose-Einstein condensate*, Commun. Pure Appl. Math. **59**, no. 12, 1659 (2006)

[12] S. Fournais, J.P. Solovej, *The energy of dilute Bose gases*, Annals of Mathematics **192**, 893 (2020)

[13] S. Fournais, J.P. Solovej, *The energy of dilute Bose gases II: The general case*, arXiv:2108.12022v2 [math-ph] (2021)

[14] K. Huang, *Statistical Mechanics*, Second edition, John Wiley & Sons, Inc., New York (1987)

[15] K. Huang, C.N. Yang, Phys. Rev. **105**, 767 (1957)

[16] E.H. Lieb, M. Loss, *Analysis, 2nd Ed.*, AMS, Providence, Rhode Island (2010)

[17] E.H. Lieb, *Simplified Approach to the Ground State Energy of an Imperfect Bose Gas*, Phys. Rev. **130**, 2518 (1963)

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

[19] E.H. Lieb, R. Seiringer, J. Yngvason, *Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional*, Phys. Rev. A **61**, 043602 (2000)

[20] E.H. Lieb, J. Yngvason, *Ground State Energy of the Low Density Bose Gas*, Phys. Rev. Lett. **80**, 2504 (1998)

[21] M. Reed, B. Simon, *Methods of modern mathematical physics I, Functional Analysis*, Academic Press, San Diego (1980)

[22] R. Seiringer, *Free Energy of a Dilute Bose Gas: Lower Bound*, Commun. Math. Phys. **279**, 595 (2008)

[23] R. Seiringer: *The thermodynamic pressure of a dilute Fermi gas*, Commun. Math. Phys. **261**, 729 (2006)

[24] J. P. Solovej, *Many Body Quantum Mechanics*, URL: `http://web.math.ku.dk/~solovej/MANYBODY/mbnotes-ptn-5-3-14.pdf` (2014)

[25] J.P. Solovej, *Upper Bounds to the Ground State Energies of the One- and Two-Component Charged Bose Gases*, Commun. Math. Phys. **266**, 797 (2006).

[26] A. Sütő, *Correlation inequalities for noninteractin Bose gases*, J. Phys. A: Math. Gen. **37**, 3 (2004)

[27] S. Sutter, *Correlation Energy in the Mean-Field Regime for a Fermionic System*, Master thesis, UZH, unpublished (2021)

[28] W. Thirring, *Quantum Mathematical Physics, Atoms, Molecules and Large Systems*, Second Edition, Springer Verlag, Berlin (2004)

[29] H.-T. Yau, J. Yin, *The second order upper bound for the ground energy of a Bose gas*, J. Stat. Phys. **136**, 453 (2009)

[30] J. Yin, *Free Energies of Dilute Bose Gases: Upper Bound*, J. Stat. Phys. **141**, 683 (2010)