Master Thesis

Correlation Energy in the Mean-Field Regime for a Fermionic System

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Abstract

Hartree–Fock approximation is used to describe interacting fermions in the mean-field approximation. However, it says nothing about the correction due to many-body correlations. In this thesis we describe the correction with respect to the Hartree–Fock state given by plane waves. We give a short introduction to the second quantization formalism and to Bogoliubov transformations. This is used to describe collective particle–hole excitations. These excitations behave as almost-bosonic operators. The correlation energy can then be expressed as the ground state energy of a quadratic Hamiltonian in terms of these particle–hole excitations. We use Bogoliubov theory to construct a suitable trial state which produces an upper bound for the correlation energy. The upper bound coincides with the Gell-Mann–Brueckner formula up to an error of smaller order.

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Chapter 1

Introduction

In classical mechanics a particle is described by its position x and its momentum p. Its energy can be determined through the classical Hamiltonian

$$\mathcal{H}(x,p) = \frac{p^2}{2m} + V(x)$$

where m is the mass of the particle and $V(x)$ is the potential. The energy of an electron in the hydrogen atom (negatively charged electron moving around positively charged nuclei) described with classical mechanics is not bounded from below. By Maxwell's law the electron emits electromagnetic radiation and the energy of the electron decreases. Thus, by classical mechanics the distance of the electron and the nuclei would decrease until the electron collapses into the nuclei. At the beginning of the twentieth century this was a problem. It was known that atoms exist and they contain a positively charged nuclei with electrons moving around it but the description with classical mechanics failed.[4]
This problem was solved with the introduction of quantum mechanics, where a particle is described by a wave function $\psi \in L^2(\mathbb{R}^3)$. The function $|\psi(x)|^2$ is interpreted as the probability density for a particle being close to x. For this interpretation, we additionally need to demand the wave function to be normalized, so $\|\psi\|_2 = 1$. We notice that a statement for the exact position of a particle is not possible. We can only make a probabilistic statement. For each physical measurable quantity, an observable, there is a corresponding operator A acting on $L^2(\mathbb{R}^3)$ such that the expectation value of this observable is given by $\langle \psi, A\psi \rangle$. The operator for the energy is obtained by the first quantization of the classical Hamiltonian. The momentum variable is replaced by the differential operator $-i\hbar\nabla$ and the position variable by a multiplication operator x. This operator is called Hamilton operator and is of the form

$$H = -\frac{\hbar^2}{2m}\Delta + V(x)$$

where $V(x)$ acts as a multiplication operator on $L^2(\mathbb{R}^3)$. Of special interest is the ground state and its corresponding ground state energy. It is the eigenfunction with the smallest eigenvalue, i.e. we are interested in solving the equation $H\psi = E\psi$ for normalized ψ. An exact solution for this equation exist only for some specific choices of the potential. Examples are the hydrogen atom ($V(x) = -1/|x|$) or the harmonic oscillator ($V(x) = \omega^2 x^2$). A physical system consist of many particles interacting with each other. Such a

system is described by a wave function $\psi \in L^2(\mathbb{R}^{3N})$ where N is the number of particles. (We neglect the spin.) The Hamilton operator of such a system is given by

$$H_N = -\frac{\hbar^2}{2m} \sum_{1 \leq j \leq N} \Delta_{x_j} + \sum_{1 \leq i < j \leq N} V(x_i - x_j).$$

Moreover we need to distinguish between bosons and fermions. Bosons are described by symmetric wave functions while fermions are described by anti-symmetric wave functions. This thesis deals with a system of fermions. In general it is not possible to solve $H_N \psi = E\psi$ on $L^2_a(\mathbb{R}^{3N})$. Therefore, several approximation methods were developed. An example is Hartree–Fock theory where we restrict our attention to Slater determinants. The physical interpretation is that instead of thinking that a particle interacts with all other particles we think of all other particle creating an external field, the mean-field, which acts on the particle. So the two-body interaction is replaced by a one-body potential and the many-body problem is reduced to a one-body problem. Hartee–Fock theory is a well-established tool to approximate a system of interacting fermions but it gives no information about the correction coming from many-body correlations. The correlation energy of a system with compact supported potential is treated in [2]. An upper bound for this energy was found which agrees with the Gell-Mann–Brueckner formula up to an error of order $o(\hbar)$.

In this thesis we want to study the correlation energy for a larger class of potentials. We will show that the upper bound for the correlation energy is also valid under the assumption that the potential in momentum space has sufficient fast power decay. The structure of the thesis is given below.

In Chapter 2 we introduce the problem and give the basic preliminaries needed in this thesis. We give a short introduction to the second quantization formalism and Bogoliubov transformations.

In Chapter 3 we present our main result.

In Chapter 4 we use a Bogoliubov transformation to rewrite the problem as a minimization problem. Moreover we introduce particle–hole pairs and we show that we can combine them to construct almost bosonic operators.

In Chapter 5 we construct our trial state for the minimization problem and we give some important properties of this state.

In Chapter 6 we evaluate the energies of the trial state using the properties of the trial state showed in Chapter 5. Combining all energies, we are able to proof the modified version of the theorem.

In Chapter 7 we present the proof of the main theorem using the results of the previous chapters.

Chapter 2

Background in Quantum Mechanics

We start with a preliminary section on quantum mechanics to introduce the most basic definitions needed in the course of the following pages. Note that we restrict our attention to fermionic systems. Therefore, all definitions and statements are mainly for fermions, even though there are bosonic equivalents which are not mentioned here.

2.1 Canonical Ensemble

The aim of this section is to formally describe an N-particle system in the mean-field regime and to get familiar with the Hartree–Fock functional and the correlation energy. The material has been taken from the book of Benedikter, Porta and Schlein [1, Chapter 6] and from the paper of Benedikter, Nam, Porta, Schlein and Seiringer [2, Chapter 1].

We consider a system of $N >> 1$ fermionic particles with mass $m > 0$ in the torus $\mathbb{T}^3 = \mathbb{R}^3/(2\pi\mathbb{Z}^3)$, interacting via a two-body potential V, in the mean-field scaling regime. The Hamiltonian of this system is defined as

$$H_N := -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{x_i} + \frac{1}{N}\sum_{1\leq i<j\leq N} V(x_i - x_j), \tag{2.1}$$

where we set

$$\hbar = N^{-1/3}.$$

This choice together with the choice of the coupling constant $1/N$ guarantees that both, the kinetic and the potential energy, are of order N. The Hamiltonian acts on the Hilbert space $L^2_a\left((\mathbb{T}^3)^N\right)$, consisting of square-integrable functions that are anti-symmetric under permutation of the N arguments. The ground state energy of the system is defined as

$$E_N := \inf_{\substack{\psi\in L^2_a\left((\mathbb{T}^3)^N\right)\\ \|\psi\|=1}} \langle\psi, H_N\psi\rangle. \tag{2.2}$$

Probabilistic interpretation: Assume the system is described through the function ψ. We define $V_i := \sum_j V(x_i - x_j)$ to be the whole potential on the i-th particle. We can think

of the $V_i's$ as random variables and we assume that they are independent and identically distributed. By the law of large numbers we find that for all $\epsilon > 0$

$$\lim_{N\to\infty} \mathbb{P}\Big(\frac{1}{N}\sum_i V_i - \langle\psi, V_i\psi\rangle > \epsilon\Big) = 0$$

This means we can replace the total potential operator $\frac{1}{N}\sum_{i,j} V(x_i - x_j)$ with the operator $\frac{1}{N}\sum_i \langle\psi, V_i\psi\rangle$. The physical interpretation is that for a single particle we can replace the interaction with all other particles by the average of the interactions; the mean field. Thus, as a approximation we can replace the two-body potential with a one-body operator. Finding the ground state of the many-body operator H_N, defined in (2.1), reduces to finding the lowest N eigenstates of a one-particle operator. Building the Slater determinant of these eigenstates yields an approximate groundstate for (2.1). Therefore we can restrict our attention to Slater determinants which are the content of Hartree–Fock theory.

In Hartree–Fock theory the ground state is expected to be approximated by a Slater determinant

$$\psi_{\text{Slater}}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma\in S_N} \operatorname{sgn}(\sigma) f_1(x_{\sigma(1)}) f_2(x_{\sigma(2)}) \dots f_N(x_{\sigma(N)})$$

with $\{f_j\}_{j=1}^N$ being an orthonormal set in $L^2(\mathbb{R}^3)$. The one-particle reduced density matrix associated with ψ_{Slater} is given by

$$\omega_N = N \operatorname{tr}_{2,\dots,N} |\psi_{\text{Slater}}\rangle \langle\psi_{\text{Slater}}| = \sum_{j=1}^N |f_j\rangle \langle f_j| .$$

Notice that ω_N is the orthogonal projection onto the subspace of $L^2(\mathbb{R}^3)$ spanned by the orbitals $\{f_j\}_{j=1}^N$. The energy of a Slater determinant can be expressed in terms of the one-particle reduced density matrix ω_N, through the Hartree–Fock energy functional

$$\begin{aligned}\mathcal{E}_{\text{HF}}(\omega_N) :&= \langle\psi_{\text{Slater}}, H_N\psi_{\text{Slater}}\rangle \\ &= \operatorname{tr}\Big(\frac{-\hbar^2}{2m}\Delta\omega_N\Big) + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)\omega_N(x,x)\omega_N(y,y) \\ &\quad - \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)|\omega_N(x,y)|^2.\end{aligned}$$

The first two summands, the kinetic and direct term, are typically of order N while the third summand is of order 1 and called exchange term. Minimizing $\mathcal{E}_{\text{HF}}(\omega_N)$ over all orthogonal projections ω_N with $\operatorname{tr}\omega_N = N$ gives an upper bound for the ground state energy E_N. We define the Fermi ball

$$B_{\text{F}} := \{k \in \mathbb{Z}^3 : |k| \le k_{\text{F}}\} ,$$

where k_{F} is the Fermi momentum, such that we need N particles to fill the Fermi ball, i.e. $N := |B_{\text{F}}|$. We choose N such that this is possible and no mode is left empty. By Gauss' classical counting argument, we have

$$\begin{aligned}k_{\text{F}} = \kappa N^{1/3} , \quad \kappa = \kappa(N) &= (3/4\pi)^{1/3} + \mathcal{O}(N^{-1/3}) \\ &=: \kappa_0 + \mathcal{O}(N^{-1/3}).\end{aligned}$$

The energy $E_{\mathrm{F}} := k_{\mathrm{F}}^2/(2m)$ is called the Fermi energy, and the sphere $k_{\mathrm{F}}\mathbb{S}^2$ of radius k_{F} is called the Fermi surface.

The ground state of N non-interacting particles on the torus is given by the Slater determinant constructed from plane waves

$$f_k(x) = (2\pi)^{-3/2} e^{ik\cdot x}, \quad k \in \mathbb{Z}^3,$$

where the momenta $k_1, \dots k_N \in \mathbb{Z}^3$ are chosen to minimize the kinetic energy compatible with the Pauli principle (filling the Fermi ball up to the Fermi momentum k_{F}). We denote by ω_{pw} the reduced one-particle density matrix associated to this state,

$$\omega_{\mathrm{pw}} = \sum_{i=1}^{N} |f_{k_i}\rangle \langle f_{k_i}| .$$

It turns out that this simple state is a stationary state of the Hartree–Fock energy functional even with interactions, and in our setting provides a good approximation of the minimum of the Hartree–Fock functional. The correlation energy is defined as the difference of the ground state energy and the Hartree–Fock energy of the plane wave state, i.e. $E_N - \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}})$. The correlation energy quantifies the effect of correlations in the true many-body ground state.

2.2 Second Quantization Formalism

Sometimes it is helpful to consider all particle numbers at the same time. To describe such systems we introduce the Fock space and the second quantization formalism. It allows us to describe systems with an unknown number of particles but we will see that it is also useful for proving statements about systems with a fixed number of particles. The theory of this section is mainly taken from Chapter 6 and 7 of the lecture notes by Solovej [5]. Additional material has been taken from Saffirio [3, Chapter 2].

We start by introducing the Fock space on a general Hilbert space $\mathcal{H}$.

Definition 2.1. *The Fock space $\mathcal{F}$ or $\mathcal{F}(\mathcal{H})$ built on the single-particle Hilbert space $\mathcal{H}$ is defined as*

$$\mathcal{F} := \mathbb{C} \bigoplus_{N\geq 1} \mathcal{H}^{\otimes N}.$$

The vector $1 \in \mathbb{C}$ is often called the vacuum vector and is denoted by Ω.

The Fock space consists of infinite sequences where the N-th term describes an N-particle state. The restriction of an N-particle state gives $\mathcal{H}^{\otimes N}$. So the definition coincides with the description of the canonical ensemble. Since we are interested in a system of fermions, which are described by anti-symmetric wave functions, we need to restrict the Fock space to these kind of functions. In order to do so, we need the following projection.

Definition 2.2. [5, Chapter 1] *We define the projection $P_- : \mathcal{H}^{\otimes N} \to \mathcal{H}^{\otimes N}$ by*

$$P_- = (N!)^{-1} \sum_{\sigma\in S_N} \mathrm{sgn}(\sigma) U_\sigma$$

where $U_\sigma : \mathcal{H}^{\otimes N} \to \mathcal{H}^{\otimes N}$ *acts on on a pure tensor product as*

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

This projection is used to define the fermionic Fock space $\mathcal{F}^{\mathrm{F}}(\mathcal{H}) := P_-(\mathcal{F}(\mathcal{H}))$. If we have an operator A on $\mathcal{H}$ we need to lift A to the Fock space. To do so, we introduce the second quantization of a one-particle operator.

Definition 2.3. *Let A be a one-particle operator. The second quantization of A, denoted by $\mathrm{d}\Gamma(A)$, is defined as*

$$\mathrm{d}\Gamma(A) := \bigoplus_{N=1}^{\infty} A_N$$

where $A_N := \sum_{j=1}^{N} \mathbb{I}^{\otimes j-1} \otimes A \otimes \mathbb{I}^{\otimes N-j}$ *acts on the N-particle sector.*

An example of the second quantization of an operator is the number of particle operator $\mathcal{N} = \mathrm{d}\Gamma(\mathbb{I})$. It acts on the N-particle sector of $\mathcal{F}$ as a multiplication with N. Since the potential acts on two particles we also need to lift two-particle operators to the Fock space. This can be done similarly to the case of one-particle operators.

Definition 2.4. *Let A be a two-body operator and let X_{ij} be the operator, obtained by exchanging the i-th particle with the first one, the j-th particle with the second and letting all other particles invariant. The second quantization of A is defined as*

$$\mathrm{d}\Gamma(A) = \bigoplus_{N=2}^{\infty} A_N$$

where $A_N := \sum_{1 \le i < j \le N} X_{ij}(A \otimes \mathbb{I}^{\otimes N-2})X_{ij}$.

If we consider all particle numbers at the same time, we call it the grand canonical picture.

An important tool in studying many body systems on the Fock space is the creation and annihilation operator.

Definition 2.5. *For $f \in \mathcal{H}$ we define the creation operator $a^*(f) : \mathcal{F} \to \mathcal{F}$ by the action on pure tensor product of the N-th sector*

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

The annihilation operator $a(f)$ is defined by

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

They act on the 0-particle space $\mathbb{C}$ as $a^*(f)\Omega = f$ and $a(f)\Omega = 0$.

We can think of $a^*(f)$ as creating a particle in the one-particle state f and $a(f)$ as annihilating a particle in this state. Since we consider a fermionic system, we need to define the creation and annihilation operator also on the fermionic Fock space. The annihilation operator is simply restricted to the fermionic subspace. This does not work for the creation operator because the image contains non-anti-symmetric functions. We need to project back onto the anti-symmetric subspace. Thus, on the fermionic Fock space $\mathcal{F}^{\mathrm{F}}$ we define the fermionic annihilation and creation operator as

$$a_-(f) := a(f), \quad a_-^*(f) := P_- a^*(f).$$

The next lemmas show some important properties of the fermionic creation and annihilation operator.

Lemma 2.1. *Creation and annihilation operator are the adjoint from each other, i.e.* $a_-^*(f) = (a_-(f))^*$.

Proof. Let $g_1 \otimes \ldots \otimes g_{N-1}$ and $h_1 \otimes \ldots \otimes h_N$ be pure tensor products of the $(N-1)$-th and N-th sector of $\mathcal{F}$. Additionally, let $g_N \in \mathcal{H}$. We compute

$$\begin{aligned}
&\langle P_- a^*(g_N) g_1 \otimes \ldots \otimes g_{N-1}, h_1 \otimes \ldots \otimes h_N \rangle \\
=&N^{1/2} \langle P_- g_N \otimes g_1 \otimes \ldots \otimes g_{N-1}, h_1 \otimes \ldots \otimes h_N \rangle \\
=&\frac{1}{N!} N^{1/2} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \langle g_{\sigma^{-1}(N)} \otimes g_{\sigma^{-1}(1)} \otimes \ldots \otimes g_{\sigma^{-1}(N-1)}, h_1 \otimes \ldots \otimes h_N \rangle \\
=&\frac{1}{N!} N^{1/2} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \langle g_N \otimes g_1 \otimes \ldots \otimes g_{N-1}, h_{\sigma^{-1}(1)} \otimes \ldots \otimes h_{\sigma^{-1}(N)} \rangle \\
=&\frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \langle g_1 \otimes \ldots \otimes g_{N-1}, N^{1/2} \langle g_N, h_{\sigma^{-1}(1)} \rangle h_{\sigma^{-1}(2)} \otimes \ldots \otimes h_{\sigma^{-1}(N)} \rangle \\
=&\frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \langle g_1 \otimes \ldots \otimes g_{N-1}, a(g_N) h_{\sigma^{-1}(1)} \otimes \ldots \otimes h_{\sigma^{-1}(N)} \rangle \\
=&\langle g_1 \otimes \ldots \otimes g_{N-1}, a(g_N) P_- h_1 \otimes \ldots \otimes h_N \rangle
\end{aligned}$$

By bilinearity we get that for for every $g, h \in \mathcal{F}$ and $f \in \mathcal{H}$

$$\langle P_- a^*(f) g, h \rangle = \langle g, a(f) P_- h \rangle \tag{2.3}$$

In particular, the equality (2.3) holds on the fermionic Fock space and we conclude $a_-^*(f) = (a(f))^*$. □

Lemma 2.2. *The map $f \to a_-^*(f)$ is linear whereas the map $f \to a_-(f)$ is anti-linear.*

Proof. The claim follows directly from the definition of the creation and annihilation operator [see Definition 2.5]. □

Lemma 2.3 (Canonical Anti-Commutation Relation)**.** *The creation and annihilation operator satisfy the Canonical Anti-Commutation Relation (CAR)*

$$\{a_-(f), a_-(g)\} = 0 = \{a_-^*(f), a_-^*(g)\}, \quad \textit{and} \quad \{a_-(f), a_-^*(g)\} = \langle f, g \rangle. \tag{2.4}$$

Proof. For a pure tensor $h_1 \otimes \ldots \otimes h_N$ we compute

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

We conclude that $\{a_-(f), a_-(g)\} = 0$.

Similarly, we compute for the fermionic creation operator

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

We conclude that $\{a_-^*(f), a_-^*(g)\} = 0$.

For the anti-commutator of $a_-(f)$ with $a_-^*(g)$ we compute $a_-(f)a_-^*(g)$ and $a_-^*(g)a_-(f)$ acting on a anti-symmetrized pure tensor $P_-g_1 \otimes \ldots \otimes g_{N-1}$. For simpler notation we write g_N instead of g. We get

$$\begin{aligned}
&a_-(f)a_-^*(g_N)P_-g_1 \otimes \ldots \otimes g_{N-1} = a(f)P_-a^*(g_N)g_1 \otimes \ldots \otimes g_{N-1} \\
=&\frac{1}{(N-1)!}\sum_{\sigma\in S_N} \mathrm{sgn}(\sigma)\langle f, g_{\sigma^{-1}(N)}\rangle g_{\sigma^{-1}(1)} \otimes \ldots \otimes g_{\sigma^{-1}(N-1)} \\
=&\frac{1}{(N-1)!}\sum_{\substack{\sigma\in S_N \\ \sigma(N)\neq N}} \mathrm{sgn}(\sigma)\langle f, g_{\sigma^{-1}(N)}\rangle g_{\sigma^{-1}(1)} \otimes \ldots \otimes g_{\sigma^{-1}(N-1)} \\
&+\frac{1}{(N-1)!}\sum_{\substack{\sigma\in S_N \\ \sigma(N)= N}} \mathrm{sgn}(\sigma)\langle f, g_N\rangle g_{\sigma^{-1}(1)} \otimes \ldots \otimes g_{\sigma^{-1}(N-1)} \\
=&-\frac{1}{(N-1)!}\sum_{\substack{\sigma\in S_N \\ \sigma(N)\neq 1}} \mathrm{sgn}(\sigma)\langle f, g_{\sigma^{-1}(1)}\rangle g_{\sigma^{-1}(N)} \otimes g_{\sigma^{-1}(2)} \otimes \ldots \otimes g_{\sigma^{-1}(N-1)} \qquad (2.5) \\
&+\langle f, g_N\rangle P_-g_1 \otimes \ldots \otimes g_{N-1}.
\end{aligned}$$

We proved the claim for anti-symmetrized pure tensors if we show that the first summand in (2.5) equals to $-a_-^*(g_N)a_-(f)P_-g_1 \otimes \ldots \otimes g_{N-1}$. For this purpose, we compute

$$\begin{aligned}
&a_-^*(g_N)a_-(f)P_-g_1 \otimes \ldots \otimes g_{N-1} = P_-a^*(g_N)a(f)P_-g_1 \otimes \ldots \otimes g_{N-1} \\
=&\frac{N-1}{[(N-1)!]^2}\sum_{\sigma,\pi\in S_{N-1}} \mathrm{sgn}(\sigma)\mathrm{sgn}(\pi)\langle f, g_{\sigma^{-1}(1)}\rangle g_{\pi^{-1}(N)} \otimes g_{\pi^{-1}\sigma^{-1}(2)} \otimes \ldots \otimes g_{\pi^{-1}\sigma^{-1}(N-1)}
\end{aligned}$$

where for fixed σ the permutation π acts on the elements $N, \sigma^{-1}(2), \dots \sigma^{-1}(N-1)$. Now we are going to consider σ and π as a permutation in S_N mapping N and $\sigma^{-1}(1)$ respectively to itself. We get

$$\frac{N-1}{[(N-1)!]^2} \sum_{\substack{\sigma,\pi\in S_N \\ \pi^{-1}\sigma^{-1}(1)=\sigma^{-1}(1)}} \operatorname{sgn}(\sigma\circ\pi)\langle f, g_{\pi^{-1}\sigma^{-1}(1)}\rangle \\ \times g_{\pi^{-1}\sigma^{-1}(N)} \otimes g_{\pi^{-1}\sigma^{-1}(2)} \otimes \dots \otimes g_{\pi^{-1}\sigma^{-1}(N-1)}$$

We combine π and σ to a permutation in S_N. More precisely, we define the composition $\tilde{\sigma} := \sigma \circ \pi$. Note that σ (as a permutation in S_N) maps N to itself and the preimage of 1 will never be N. Thus, the condition $\pi^{-1}\sigma^{-1}(1) = \sigma^{-1}(1)$ translates to $\tilde{\sigma}^{-1}(1) \neq N$. Additionally, for every permutation $\tilde{\sigma} \in S_N$ with $\tilde{\sigma}^{-1}(1) \neq N$ we have exactly $(N-2)!$ possibilities to compose permutations $\sigma, \pi \in S_N$ in order to get $\tilde{\sigma}$ with $\pi(\sigma^{-1}(1)) = \sigma^{-1}(1)$ and $\sigma(N) = N$. This means each permutation $\tilde{\sigma}$ appears $(N-2)!$ times in the sum over $\sigma, \pi \in S_N$. Therefore we need to multiply the expression with $(N-2)!$. We find

$$= \frac{1}{(N-1)!} \sum_{\substack{\tilde{\sigma}\in S_N \\ \tilde{\sigma}^{-1}(1)\neq N}} \operatorname{sgn}(\tilde{\sigma})\langle f, g_{\tilde{\sigma}^{-1}(1)}\rangle g_{\tilde{\sigma}^{-1}(N)} \otimes g_{\tilde{\sigma}^{-1}(2)} \otimes \dots g_{\tilde{\sigma}^{-1}(N-1)}$$

which is equal to the first summand in the last line of (2.5). Thus, we conclude that $\{a_-(f), a_-^*(g)\} = \langle f, g\rangle$ on anti-symmetrized pure tensors. By linearity we can expand the claim to all elements in the fermionic Fock space. This proves the statement. □

Often it is helpful to write the second quantization of an operator in terms of creation and annihilation operator. The following two lemmas give an alternative writing of $\mathrm{d}\Gamma(A)$ for a one- and a two-particle operator A.

Lemma 2.4 (Second Quantization of 1-Body Operators)**.** *Let A be a symmetric operator on $\mathcal{H}$ and let $\{f_\alpha\}_{\alpha=1}^\infty$ be an orthonormal basis for $\mathcal{H}$ with elements from the domain $D(A)$. The second quantization of A on the fermionic Fock space is*

$$\mathrm{d}\Gamma(A) = \sum_{\beta=1}^\infty \sum_{\alpha=1}^\infty \langle f_\alpha, Af_\beta\rangle a_-^*(f_\alpha) a_-(f_\beta)$$

as quadratic forms on the domain $\cup_{M=0}^\infty \bigoplus_{N=1}^M P_- D(A_N)$.

Proof. First, recall that since $\{f_\alpha\}_{\alpha=1}^\infty$ is a orthonormal basis we can express each $g \in \mathcal{H}$ as

$$g = \sum_{\alpha=1}^\infty \langle f_\alpha, g\rangle f_\alpha.$$

It follows that if $g, h \in D(A)$ then

$$\sum_{\beta=1}^\infty \sum_{\alpha=1}^\infty \langle g, f_\alpha\rangle\langle f_\alpha, Af_\beta\rangle\langle f_\beta, h\rangle = \sum_{\beta=1}^\infty \langle g, Af_\beta\rangle\langle f_\beta, h\rangle = \sum_{\beta=1}^\infty \langle Ag, f_\beta\rangle\langle f_\beta, h\rangle \\ = \langle Ag, h\rangle = \langle g, Af\rangle.$$

The action of $a^*(f_\alpha)a(f_\beta)$ on a pure tensor is

$$a^*(f_\alpha)a(f_\beta)\varphi_1 \otimes \ldots \otimes \varphi_N = N\langle f_\beta, \varphi_1\rangle f_\alpha \otimes \varphi_2 \otimes \ldots \otimes \varphi_N$$

where $\varphi_1, \ldots \varphi_N \in D(A)$. Thus we get

$$\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty}\langle f_\alpha, Af_\beta\rangle a^*(f_\alpha)a(f_\beta) = N(A \otimes \mathbb{I}^{\otimes N-1})$$

as quadratic forms on finite linear combinations of N-fold pure tensor products of vectors from $D(A)$.

Since P_- projects onto anti-symmetrized vectors we have on $\mathcal{H}^{\otimes N}$

$$P_- N(A \otimes \mathbb{I}^{\otimes N-1})P_- = P_- \sum_{j=1}^{N} A^{(j)} P_- = \sum_{j=1}^{N} A^{(j)} P_-$$

where $A^{(j)} = \mathbb{I}^{\otimes j-1} \otimes A \otimes \mathbb{I}^{\otimes N-j}$. We conclude that

$$\begin{aligned}\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty}\langle f_\alpha, Af_\beta\rangle a_-^*(f_\alpha)a_-(f_\beta)P_- &= \sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty}\langle f_\alpha, Af_\beta\rangle P_- a^*(f_\alpha)a(f_\beta)P_- \\ &= \bigoplus_{N=1}^{\infty}\sum_{j=1}^{N} A^{(j)}P_- = \mathrm{d}\Gamma(A).\end{aligned}$$

□

Lemma 2.5 (Second Quantization of 2-Body Operators)**.** *Let V be a 2-body potential for identical particles (a symmetric operator on $\mathcal{H} \otimes \mathcal{H}$ such that $WVW = V$ where W is the unitary exchange operator). Let $\{f_\alpha\}_{\alpha=1}^{\infty}$ be an orthonormal basis for $\mathcal{H}$ such that $f_\alpha \otimes f_\beta \in D(V)$ for all $\alpha, \beta = 1, 2, \ldots$. Then as quadratic forms on finite linear combinations of pure anti-symmetric tensor products of basis vectors from $\{f_\alpha\}_{\alpha=0}^{\infty}$ we have*

$$\mathrm{d}\Gamma(V) = \frac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1}^{\infty}\langle f_\alpha \otimes f_\beta, Vf_\mu \otimes f_\nu\rangle a_-^*(f_\alpha)a_-^*(f_\beta)a_-(f_\nu)a_-(f_\mu).$$

Proof. Since $\{f_\alpha\}_{\alpha=1}^{\infty}$ is an orthonormal basis we have

$$V(f_1 \otimes f_2) = \sum_{\alpha,\beta,\mu,\nu=1}^{\infty}\langle f_\alpha \otimes f_\beta, Vf_\mu \otimes f_\nu\rangle\langle f_\mu, f_1\rangle\langle f_\nu, f_2\rangle f_\alpha \otimes f_\beta \tag{2.6}$$

and

$$a^*(f_\alpha)a^*(f_\beta)a(f_\nu)a(f_\mu)f_1 \otimes \ldots \otimes f_N = N(N-1)\langle f_\mu, f_1\rangle\langle f_\nu, f_2\rangle f_\alpha \otimes f_\beta \otimes f_3 \otimes \ldots \otimes f_N.$$

Since this is true for any N-fold pure tensor product of basis vectors and together with (2.6) we conclude that on such tensor products it holds

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

where $V_{12}=V\otimes\mathbb{I}^{\otimes N-2}$. As in the proof of the second quantization of the one-body operator, we have that on N-fold tensor products

$$\frac{N(N-1)}{2}P_-W_{12}P_-=\sum_{1\leq i<j\leq N}V_{ij}P_-.$$

Here we used that $WVW=V$ and that V_{ij} is the operator acting on the i-th and j-th particle with V and on the other particles with the identity. If we anti-symmetrize after creating a particle it is irrelevant whether we have anti-symmetrized before or not. Therefore, we have $P_-a^*(f)P_-=P_-a^*(f)$ and thus

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

□

For simplicity, from now on we denote the fermionic Fock space by $\mathcal{F}$ and its creation and annihilation operator by a^* and a.

For $\mathcal{H}=L^2(\mathbb{T}^3)$ we can express the creation and annihilation operator also in terms of operator valued distributions a_x^* and a_x, creating or annihilating a fermionic particle at $x\in\mathbb{T}^3$,

$$\begin{aligned}
a_x^*&=\sum_{k\in\mathbb{Z}^3}e^{ik\cdot x}a_k^*\\
a_x&=\sum_{k\in\mathbb{Z}^3}e^{-ik\cdot x}a_k
\end{aligned}\tag{2.7}$$

where $a_k^*=a^*((2\pi)^{-3/2}e^{ik\cdot x})$. Using the expressions above we find

$$\int f(x)a_x^*\mathrm{d}x=\sum_{k\in\mathbb{Z}^3}\int \mathrm{d}x f(x)e^{ik\cdot x}a_k^*=a^*(f)$$

and similarly

$$\int \overline{f(x)} a_x \mathrm{d}x = a(f).$$

The operators a_x^* and a_x also satisfy the usual canonical anti-commutation relation,

$$\{a_x, a_y\} = 0 = \{a_x^*, a_y^*\},\ \{a_x, a_y^*\} = \delta(x-y). \tag{2.8}$$

If an operator A has an integral kernel $A(x;y)$, the second quantization of A is given by

$$\mathrm{d}\Gamma(A) = \int A(x,y) a_x^* a_y \mathrm{d}x \mathrm{d}y.$$

This formula is not useful for the Hamilton operator. To write the second quantization of the Hamiltonian in terms of a_x and a_x^* we use the formulas in the Lemmas 2.4 and 2.5 and the expression for a_x^* and for a_x in (2.7). Then we find that the second quantization of the Hamiltonian, defined in (2.1), can be written as [2, Section 3.1]

$$\mathrm{d}\Gamma(H_N) = \frac{\hbar^2}{2m} \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \int \mathrm{d}x \mathrm{d}y V(x-y) a_x^* a_y^* a_y a_x. \tag{2.9}$$

The next lemma collects some useful bounds.

Lemma 2.6 (Standard Bounds for the Second Quantization of an Operator)**.** *Let A be a bounded operator on $\mathcal{H}$. Then for every $\Psi \in \mathcal{F}$,*

$$\begin{aligned} \langle \Psi, \mathrm{d}\Gamma(A)\Psi \rangle &\leq \|A\|_{\mathrm{op}} \langle \Psi, \mathcal{N}\Psi \rangle, \\ \|\mathrm{d}\Gamma(A)\Psi\| &\leq \|A\|_{\mathrm{op}} \|\mathcal{N}\Psi\|. \end{aligned}$$

Proof. To prove the first inequality we note that it is sufficient to prove the claim for pure tensor products on the N-th sector. We have

$$\begin{aligned} &\langle g_1 \otimes \ldots \otimes g_N, \sum_{j=1}^N A_N g_1 \otimes \ldots \otimes g_N \rangle \\ =&\sum_{j=1}^N \langle g_1 \otimes \ldots \otimes g_N, (\mathbb{I}^{\otimes j-1} \otimes A \otimes \mathbb{I}^{\otimes N-j}) g_1 \otimes \ldots \otimes g_N \rangle \\ =&\sum_{j=1}^N \langle g_j, A g_j \rangle \prod_{\substack{l=1 \\ l \neq j}}^N \langle g_l, g_l \rangle \leq \|A\|_{\mathrm{op}} \sum_{j=1}^N \prod_{l=1}^N \langle g_l, g_l \rangle \\ =&\|A\|_{\mathrm{op}} N \langle g_1 \otimes \ldots \otimes g_N, g_1 \otimes \ldots \otimes g_N \rangle = \|A\|_{\mathrm{op}} \langle g_1 \otimes \ldots \otimes g_N, \mathcal{N} g_1 \otimes \ldots \otimes g_N \rangle \end{aligned}$$

and we conclude the claim.
For the second inequality we show that $\|\mathrm{d}\Gamma(A)\Psi\|^2 \leq \|A\|_{\mathrm{op}}^2 \|\mathcal{N}\Psi\|^2$ for pure tensor prod-

ucts on the N-th sector. We find

$$\begin{aligned}
&\langle A_N g_1 \otimes \ldots \otimes g_N, A_N g_1 \otimes \ldots \otimes g_N \rangle \\
=&\sum_{i,j=1}^{N} \langle \mathbb{I}^{\otimes i-1} \otimes A \otimes \mathbb{I}^{\otimes N-i} g_1 \otimes \ldots \otimes g_N, \mathbb{I}^{\otimes j-1} \otimes A \otimes \mathbb{I}^{\otimes N-j} g_1 \otimes \ldots \otimes g_N \rangle \\
=&\sum_{\substack{i,j=1 \\ i \neq j}}^{N} \langle g_j, Ag_j \rangle \langle Ag_i, g_i \rangle \prod_{\substack{l=1 \\ l \neq i \\ l \neq j}}^{N} \langle g_l, g_l \rangle + \sum_{j=1}^{N} \langle Ag_j, Ag_j \rangle \prod_{\substack{l=1 \\ l \neq j}}^{N} \langle g_l, g_l \rangle \\
\leq& \|A\|_{\mathrm{op}}^2 \sum_{i,j=1}^{N} \prod_{l=1}^{N} \langle g_l, g_l \rangle = \|A\|_{\mathrm{op}}^2 N^2 \langle g_1 \otimes \ldots \otimes g_N, g_1 \otimes \ldots \otimes g_N \rangle \\
=& \|A\|_{\mathrm{op}}^2 \, \|\mathcal{N} g_1 \otimes \ldots \otimes g_N\|^2.
\end{aligned}$$

This finishes the proof of the lemma. □

Having the composition of several creation and annihilation operators it is useful to define the normal ordering.

Definition 2.6. [1, Chapter 5] *A composition of creation and annihilation operators is said to be in normal order if all creation operators are on the left side of the annihilation operators, i.e. are of the form*

$$a^*(f_1) \ldots a^*(f_n) a(g_1) \ldots a(g_m).$$

2.3 Bogoliubov Transformation

This section serves as an introduction to Bogoliubov transformations. The advantage of an Bogoliubov transformation is that it preserves the canonical (anti-)commutation relation. We will use a fermionic Bogoliubov transformation to write the correlation energy as the ground state energy of a Hamiltonian. Later we will make use of a bosonic Bogoliubov transformation to define a trial state. The definitions and results in this section are based on [5, Section 8.2 and Chapter 9] and [3, Chapter 2].

To introduce Bogoliubov transformations we need to define generalized annihilation and creation operators. Note that $J : \mathcal{H} \to \mathcal{H}^*$ is the conjugate linear map such that $Jg(f) = \langle g, f \rangle$.

Definition 2.7. *The generalized fermonic annihilation and creation operators A_- and A_-^* are defined as*

$$\begin{aligned}
A_-(f \oplus Jg) &= a_-(f) + a_-^*(g) \\
A_-^*(f \oplus Jg) &= a_-^*(f) + a_-(g).
\end{aligned}$$

A_- is a conjugate linear map from $\mathcal{H} \oplus \mathcal{H}^*$ to operators on $\mathcal{F}^{\mathrm{F}}(\mathcal{H})$ and A_-^* is a linear map. We have the relation

$$A_-^*(F) = A_-(\mathcal{J}F) \quad \text{where } \mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix} : \mathcal{H} \oplus \mathcal{H}^* \to \mathcal{H} \oplus \mathcal{H}^* \tag{2.10}$$

for all $F \in \mathcal{H} \oplus \mathcal{H}^*$. The generalized annihilation and creation operators also satisfy the canonical anti-commutation relation

$$\{A_-(F_1), A_-^*(F_2)\} = \langle F_1, F_2 \rangle_{\mathcal{H}\oplus\mathcal{H}^*} \tag{2.11}$$

but in general we have

$$\{A_-(F_1), A_-(F_2)\} \neq 0.$$

Definition 2.8. *A fermionic Bogoliubov map is a linear bounded isomorphism $\mathcal{V} : \mathcal{H} \oplus \mathcal{H}^* \to \mathcal{H} \oplus \mathcal{H}^*$ with $A_-^*(\mathcal{V}F) = A_-(\mathcal{V}\mathcal{J}F)$ for all $F \in \mathcal{H} \oplus \mathcal{H}^*$ and*

$$\{A_-(\mathcal{V}F_1), A_-^*(\mathcal{V}F_2)\} = \langle F_1, F_2 \rangle_{\mathcal{H}\oplus\mathcal{H}^*}$$

for all $F_1, F_2 \in \mathcal{H} \oplus \mathcal{H}^*$. If $\mathcal{V}$ is a Bogoliubov map then the operator transformation $A_-(F) \to A_-(\mathcal{V}F)$ is called Bogoliubov transformation.

Using (2.10) and (2.11) we may rewrite the condition for being a fermionic Bogoliubov map as

$$\langle \mathcal{V}F_1, \mathcal{V}F_2 \rangle_{\mathcal{H}\oplus\mathcal{H}^*} = \langle F_1, F_2 \rangle_{\mathcal{H}\oplus\mathcal{H}^*}, \quad \text{and} \quad \mathcal{J}\mathcal{V}F = \mathcal{V}\mathcal{J}F$$

for all $F, F_1, F_2 \in \mathcal{H} \oplus \mathcal{H}^*$. In particular, $\mathcal{V}$ is a unitary map, i.e.

$$\mathcal{V}^{-1} = \mathcal{V}^*$$

We obtain the following equivalent characterization of Bolgoliubov maps.

Theorem 2.7 (Bogoliubov Maps)**.** *A linear map $\mathcal{V} : \mathcal{H} \oplus \mathcal{H}^* \to \mathcal{H} \oplus \mathcal{H}^*$ is a fermionic Bogoliubov map if and only if*

$$\mathcal{V}^*\mathcal{V} = \mathcal{V}\mathcal{V}^* = \mathbb{I}_{\mathcal{H}\oplus\mathcal{H}^*}, \quad \textit{and} \quad \mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}. \tag{2.12}$$

We can describe a Bogoliubov map $\mathcal{V}$ by a 2×2 block matrix. From the condition $\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}$ it follows that the matrix needs to be of the form

$$\mathcal{V} = \begin{pmatrix} U & J^*VJ^* \\ V & JUJ^* \end{pmatrix} \tag{2.13}$$

where $U : \mathcal{H} \to \mathcal{H}$ and $V : \mathcal{H} \to \mathcal{H}^*$. From (2.12) we find the following relations on the maps U and V

$$U^*U = \mathbb{I} - V^*V, \quad UU^* = \mathbb{I} - J^*VV^*J, \quad JV^*JU = -JU^*J^*V. \tag{2.14}$$

Under certain conditions, a Bogoliubov transformation can be implemented by a unitary map on the Fock space $\mathcal{F}^{\mathrm{F}}$. This is the content of the next theorem. The proof can be found in [5].

Theorem 2.8 (Unitary Bogoliubov Implementation)**.** *If $\mathcal{V} : \mathcal{H} \oplus \mathcal{H}^* \to \mathcal{H} \oplus \mathcal{H}^*$ is a fermionic Bogoliubov map of the Form* (2.13) *then there exists a unitary transformation*

$$\mathbb{U}_{\mathcal{V}} : \mathcal{F}^{\mathrm{F}}(\mathcal{H}) \to \mathcal{F}^{\mathrm{F}}(\mathcal{H})$$

such that

$$\mathbb{U}_{\mathcal{V}} A_-(F) \mathbb{U}_{\mathcal{V}}^* = A_-(\mathcal{V}F)$$

for all $F \in \mathcal{H} \oplus \mathcal{H}^*$ if and only if V^*V is trace class. This condition is known as Shale-Stinespring condition. We say that the Bogoliubov transformation $\mathcal{V}$ is implementable on the fermionic Fock space.

An important property of a implementor $\mathbb{U}_{\mathcal{V}}$ is that the conjugated creation and annihilation operators $\mathbb{U}_{\mathcal{V}}^* a^*(f) \mathbb{U}_{\mathcal{V}}$ and $\mathbb{U}_{\mathcal{V}}^* a(g) \mathbb{U}_{\mathcal{V}}$ still satisfy the canonical anti-commutation relations.

By Riesz's Representation Theorem we know that we can think of the dual $\mathcal{H}^*$ as $\mathcal{H}$. Then the Bogoliubov transformation is a unitary linear map

$$\mathcal{V} : \mathcal{H} \oplus \mathcal{H} \to \mathcal{H} \oplus \mathcal{H}$$

of the form

$$\mathcal{V} = \begin{pmatrix} U & \overline{V} \\ V & \overline{U} \end{pmatrix} \tag{2.15}$$

where $U, V : \mathcal{H} \to \mathcal{H}$ are linear maps such that

$$\begin{aligned} U^*U + V^*V &= \mathbb{I}, \\ U^*\overline{V} + V^*\overline{U} &= 0. \end{aligned} \tag{2.16}$$

The properties (2.16) are the equivalent of (2.14). The generalized annihilation and creation operators on $\mathcal{H} \oplus \mathcal{H}$ act as

$$\begin{aligned} A_-(f \oplus g) &= a_-(f) + a_-^*(\bar{g}) \\ A_-^*(f \oplus g) &= a_-^*(f) + a_-(\bar{g}). \end{aligned}$$

for every $f \oplus g \in \mathcal{H} \oplus \mathcal{H}$. One can check that $\mathcal{V}$ is implementable by $\mathbb{U}_{\mathcal{V}}$ if for all $f, g \in \mathcal{H}$ it holds [1, Chapter 5]

$$\mathbb{U}_{\mathcal{V}}(a_-(f) + a_-^*(\bar{g})) \mathbb{U}_{\mathcal{V}}^* = A_-(\mathcal{V}(f \oplus g)). \tag{2.17}$$

A Slater determinant on the Fock space $\mathcal{F}$ is given by

$$a^*(f_1) \dots a^*(f_N)\Omega = \left\{0, \dots, 0, \frac{1}{\sqrt{N!}} \det(f_i(x_j))_{1 \le i,j \le N}, 0, \dots, 0\right\} \tag{2.18}$$

where $\{f_j\}_{j=1,\dots,N}$ is an orthonormal system on $\mathcal{H}$ and Ω is the vacuum state. This state has a remarkable structure: it can be obtained as an action of a Bogoliubov transformation on the vacuum state Ω. We want to show that there is a Bogoliubov transformation such that the action on the vacuum state Ω gives a Slater determinant (2.18). We consider the orthogonal projection into the N-dimensional space spanned by $f_1, \dots, f_N$

$$\omega_N = \sum_{i=1}^{N} |f_i\rangle \langle f_i| .$$

We choose

$$U_N = \mathbb{I} - \omega_N \quad \text{and} \quad V_N = \sum_{i=1}^{N} |\overline{f_i}\rangle \langle f_i|$$

for the Bogoliubov transformation $\mathcal{V}_N$ of the Form (2.15). One can easily check that U_N and V_N satisfy (2.16). Indeed, $\mathcal{V}_N$ is a Bogoliubov transformation. Since V_N is a Hilbert-Schmidt operator, there exists an implementor which can be seen as the particle–hole transformation

$$\mathbb{U}_N a_-^*(f_i)\mathbb{U}_N^* = \begin{cases} a_-(f_i), & i \leq N \\ a_-^*(f_i), & i > N. \end{cases}$$

Then the vacuum state transforms to the Slater determinant (2.18)

$$\mathbb{U}_N \Omega = a_-^*(f_1) \dots a_-^*(f_i)\Omega.$$

The map $\mathbb{U}_N$ describes fluctuations in the Slater determinant with reduced density ω_N. Creation operators act as creating a particle outside the Slater determinant or annihilating a particle inside the Slater determinant.

Let us heuristically mention why this Bogoliubov transformation is useful for our goal. The new vacuum state is the Slater determinant coming from the plane waves (choose the orthonormal system $\{f_j\}_{j=1,\dots,N}$ to be the plane waves). Recall that the correlation energy is defined as the difference of the ground state energy and the Hartree–Fock energy of the plane waves. Thus, after the transformation it is the smallest energy difference to the energy of the new vacuum state, i.e. the ground state energy of a Hamiltonian.

The next definition characterizes a special family of operators.

Definition 2.9. [5, Definition 11.1] *Let $\mathcal{A} : \mathcal{H} \oplus \mathcal{H}^* \to \mathcal{H} \oplus \mathcal{H}^*$ be a Hermitian, trace class operator and assume moreover in the bosonic case that it is positive semi-definite. An operator of the form*

$$H_{\mathcal{A}}^{\pm} = \sum_{i,j=1}^{2M} \langle F_i, \mathcal{A}F_j \rangle A_{\pm}^*(F_i) A_{\pm}(F_j),$$

where $F_1, \dots, F_{2M}$ is an orthonomal basis for $\mathcal{H} \oplus \mathcal{H}^*$ is called bosonic $(+)$ or fermionic $(-)$ quadratic Hamiltonian corresponding to $\mathcal{A}$.

Note that there is an equivalent definition for the bosonic generalized annihilation and creation operator, see [5].

Chapter 3

Main Theorem

In this chapter we present the main result of this thesis. We claim that under certain conditions on the potential we can bound the correction due to interactions from above up to an error of order smaller than $\hbar$. The theorems in this chapter are modifications of the main result in [2].

Theorem 3.1 (Upper Bound for the Ground State Energy)**.** *Let $\hat{V} : \mathbb{Z}^3 \to \mathbb{R}$ be non-negative with $\sum_{p\in\mathbb{Z}^3} \hat{V}(p)|p|^n < \infty$ for an $n > 24$. Let $k_{\mathrm{F}} > 0$ be the Fermi momentum and $N := |\{k \in \mathbb{Z}^3 : |k| \leq k_{\mathrm{F}}\}|$ be the number of particles. Recall that $\hbar = N^{-1/3}$. Let $\omega_{\mathrm{pw}} := \sum_{k\in\mathbb{Z}^3:|k|\leq k_{\mathrm{F}}} |f_k\rangle \langle f_k|$ be the projection on the filled Fermi ball. Then, asymptotically for $k_{\mathrm{F}} \to \infty$, the ground state energy (2.2) satisfies the following upper bound:*

$$\begin{aligned} E_N \leq\, & \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}}) \\ & + \frac{\hbar\kappa_0}{2m} \sum_{k\in\mathbb{Z}^3} |k| \Big[\frac{1}{\pi} \int_0^\infty \log\Big(1 + 4\pi\hat{V}(k)m\kappa_0\Big(1 - \lambda \arctan\frac{1}{\lambda}\Big)\Big) \mathrm{d}\lambda - \hat{V}(k)m\kappa_0\pi \Big] \\ & + o(\hbar) \end{aligned} \tag{3.1}$$

where $\kappa_0 = (\frac{3}{4\pi})^{1/3}$.

To prove Theorem 3.1 we are going to write our potential as a sum $V = V_{\mathrm{in}} + V_{\mathrm{out}}$ such that $\hat{V}_{\mathrm{in}}$ is supported inside a ball of radius N^μ and $\hat{V}_{\mathrm{out}}$ has support outside of this ball. The kinetic energy and the potential energy, coming from V_{in}, create the Hartree–Fock energy and the correction given by the Gell-Mann–Brueckner formula. Afterwards, we will show that the expectation value of V_{out} is sufficiently small for an appropriate choice of μ. The next theorem shows that we have a similar result for potential supported in a ball of radius N^μ.

Theorem 3.2. *Let $0 < \mu < 1/6$ and let C be a constant. Assume that $\hat{V} : \mathbb{Z}^3 \to \mathbb{R}$ is non-negative with support inside a ball of radius N^μ such that $\sum_{k\in\mathbb{Z}^3} \hat{V}(k) < C$. Let k_{F}, N, $\hbar$, and ω_{pw} be as in Theorem 3.1. Then asymptotically for $k_{\mathrm{F}} \to \infty$ and for an $0 < \epsilon < 1/3 - 2\mu$ and a $0 < \delta < 1/6 - \epsilon/2 - \mu$, the ground state energy satisfies the*

following upper bound:

$$\begin{aligned} E_N \leq\ & \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}}) \\ & + \frac{\hbar\kappa_0}{2m} \sum_{k\in\mathbb{Z}^3} |k| \Big[\frac{1}{\pi} \int_0^\infty \log\Big(1 + 4\pi\hat{V}(k) m\kappa_0 \Big(1 - \lambda \arctan\frac{1}{\lambda}\Big)\Big) \mathrm{d}\lambda - \hat{V}(k) m\kappa_0 \pi \Big] \\ & + \hbar\mathcal{O}\Big(N^{-\epsilon} + MN^{-2/3+\delta+3\mu} + N^{-\delta/2+\mu} + M^{1/4}N^{-1/6+\delta/2+\mu/2}\Big) \end{aligned} \tag{3.2}$$

with $M = N^{\frac{1}{3}+\epsilon}$.

We will use a Bogoliubov transformation to describe the correlation energy as the ground state energy of a correlation Hamiltonian and to describe collective particle–hole pair excitation. Afterwards, we will show that they behave approximately bosonic. We will see that the correlation Hamiltonian can be approximated by a quadratic Hamiltonian in terms of these particle–hole excitation. Then, we use an approximation of a bosonic Bogoliubov transformation to construct the trial state. This trial state will give the desired bound for the correlation energy. In the next chapters we are going to prove this theorem. Note that the factor $1/m$ can be factored out, replacing the potential V by mV. Therefore, only the case $m = 1$ needs to be considered. The proof is taken from [2].

Chapter 4

Collective Particle–Hole Pairs

In this chapter we will introduce the unitary particle–hole transformation. Then, the correlation energy can be represented in terms of particle–hole excitations around the Fermi surface. These particle–hole excitations behave as almost-bosonic operators. Thus, the correlation energy can be obtained by finding the ground state energy of a quadratic almost-bosonic Hamiltonian.

4.1 The Correlation Hamiltonian

We are going to describe the system on the fermionic Fock space using the results of Section 2.2. We then will use an implemented Bogoliubov transformation, as introduced in Section 2.3, such that the action on the vacuum state gives the Slater determinant constructed from plane waves. We will see that we can describe a correlation Hamiltonian in terms of the conjugated creation and annihilation operator such that its ground state energy is given by the correlation energy.

We denote by $\mathcal{F}$ the fermionic Fock space built on the single-particle space $L^2(\mathbb{T}^3)$ and by $\mathcal{H}_N$ the second quantization of the Hamilton operator H_N

$$\mathcal{H}_N = \frac{\hbar^2}{2} \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \int \mathrm{d}x \mathrm{d}y V(x-y) a_x^* a_y^* a_y a_x.$$

Recall the definition of the Fermi ball

$$B_{\mathrm{F}} := \{k \in \mathbb{Z}^3 : |k| \leq k_{\mathrm{F}}\},$$

where k_{F} is the Fermi momentum, such that we need N particles to fill the Fermi ball. We write $B_{\mathrm{F}}^{\mathrm{c}} = \mathbb{Z}^3 \setminus B_{\mathrm{F}}$ for the complement of the Fermi ball. We remind you that we obtain the filled Fermi ball by considering the Slater determinant ψ_{pw} built from the plane waves $f_{k_i}(x) = (2\pi)^{-3/2} e^{ik_i \cdot x}$, associated to the points $k_i \in B_F$, $i = 1, \ldots, N$. The reduced one-particle density matrix associated to this state is given by $\omega_{\mathrm{pw}} = \sum_{i=1}^N |f_{k_i}\rangle \langle f_{k_i}|$, i.e. the projection into the filled Fermi ball. As discussed in Section 2.3, there exists an implementation of a Bogoliubov transformation, called the unitary particle-hole transformation,

$R_{\omega_{\rm pw}} : \mathcal{F} \to \mathcal{F}$ satisfying

$$R_{\omega_{\rm pw}} a(f_k) R^*_{\omega_{\rm pw}} := \begin{cases} a(f_k) & \text{for } k \in B_F^c \\ a^*(\overline{f_k}) & \text{for } k \in B_F \end{cases} \quad \text{and} \quad R_{\omega_{\rm pw}} \Omega := \psi_{\rm pw},$$

where $\Omega = (1, 0, 0, \dots) \in \mathcal{F}$ is the vacuum vector. Recall that we used $u = \mathbb{I} - \omega_{\rm pw}$ and $v = \sum_{k \in B_{\rm F}} |\overline{f_k}\rangle \langle f_k|$ to define the Bogoliubov map. Formally writing $a_x = a(\delta(\cdot - x))$ and $\delta(y - x) = \sum_{k \in \mathbb{Z}^3} f_k(y)\overline{f_k}(x)$ and using condition (2.17) we find that the conjugated creation and annihilation operator in position space are given by

$$R_{\omega_{\rm pw}} a_x R^*_{\omega_{\rm pw}} = a(u_x) + a^*(\overline{v}_x), \quad R_{\omega_{\rm pw}} a^*_x R^*_{\omega_{\rm pw}} = a^*(u_x) + a(\overline{v}_x), \tag{4.1}$$

where $v_x(\cdot) = \sum_{k \in B_{\rm F}} \overline{f_k}(\cdot)\overline{f_k}(x)$ and $u_x(\cdot) = \delta(\cdot - x) - \sum_{k \in B_{\rm F}} f_k(\cdot)\overline{f_k}(x)$. The filled Fermi ball is the new vacuum state. The new creation operator $R_{\omega_{\rm pw}} a^*(f_k) R^*_{\omega_{\rm pw}}$ creates a hole in the Fermi ball for $k \in B_{\rm F}$ and we call momenta in $B_{\rm F}$ hole modes. For momentum $k \in B_{\rm F}^{\rm c}$, called particle mode, the operator $R_{\omega_{\rm pw}} a^*(f_k) R^*_{\omega_{\rm pw}}$ creates a particle outside the Fermi ball. For simplicity we use the notation $a^*_k := a^*(f_k)$ and to differentiate between particle and hole mode we write a^*_p for $p \in B_{\rm F}^c$ and a^*_h for $h \in B_{\rm F}$. The operator $a^*_p a^*_h$ is called particle–hole excitation.

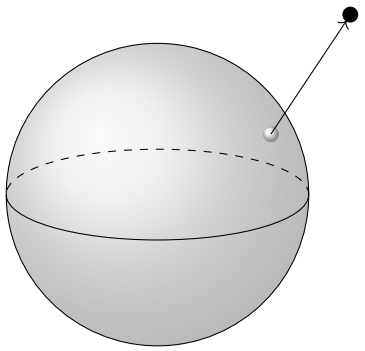

Figure 4.1: Representation of the particle-hole excitation $a^*_p a^*_h$: A particle inside the Fermi ball with momentum h is excited to a mode p outside the Fermi ball.

We introduce the number-of-particle operator $\mathcal{N}_p := \sum_{p \in B_{\rm F}^{\rm c}} a^*_p a_p$ (the particles are counted with respect to the new vacuum state) and the number-of-hole operator $\mathcal{N}_h := \sum_{p \in B_{\rm F}} a^*_h a_h$. The word fermion is used if we do not want to distinguish between holes and particles and we call $\mathcal{N} = \mathcal{N}_p + \mathcal{N}_h$ the number-of-fermion operator.

We need to compute the conjugated Hamiltonian $R^*_{\omega_{pw}} \mathcal{H}_N R_{\omega_{pw}}$. Using Relation (4.1) we find

$$R^*_{\omega_{pw}} \mathcal{H}_N R_{\omega_{pw}} = \mathcal{E}_{\rm HF}(\omega_{\rm pw}) + {\rm d}\Gamma(uhu - \overline{v}\overline{h}v) + Q_N. \tag{4.2}$$

The operator h is the one-particle Hartree–Fock Hamiltonian, given by

$$h = -\frac{\hbar^2}{2}\Delta + (2\pi)^3 \hat{V}(0) + X \tag{4.3}$$

where X is the exchange operator given by its integral kernel $X(x,y) = -N^{-1}V(x-y)\omega_{\mathrm{pw}}(x,y)$. The operator Q_N contains all contributions that are quadratic in creation and annihilation operators. It is given by

$$Q_N = \frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3} \mathrm{d}x\mathrm{d}y V(x-y)\Big(\mathcal{E}_1(x,y) + 2a^*(u_x)a^*(\overline{v}_x)a(\overline{v}_y)a(u_y) \\ + \Big[a^*(u_x)a^*(\overline{v}_x)a^*(u_y)a^*(\overline{v}_y) + \mathcal{E}_2(x,y) + \mathrm{h.c.}\Big]\Big)$$

where

$$\begin{aligned}\mathcal{E}_1(x,y) = a^*(u_x)a^*(u_y)a(u_y)a(u_x) - 2a^*(u_x)a^*(\overline{v}_y)a(\overline{v}_y)a(u_x) \\ + a^*(\overline{v}_y)a^*(\overline{v}_x)a(\overline{v}_x)a(\overline{v}_y)\end{aligned} \tag{4.4}$$

and

$$\mathcal{E}_2(x,y) = -2a^*(u_x)a^*(u_y)a^*(\overline{v}_x)a(u_y) + 2a^*(u_x)a^*(\overline{v}_y)a^*(\overline{v}_x)a(\overline{v}_y)\ . \tag{4.5}$$

Later we will show that $\mathcal{E}_1$ and $\mathcal{E}_2$ provide subleading correction to the correlation energy, as $N\to\infty$.

To proof (4.2) recall that the Hamiltonian is given by

$$\mathcal{H}_N = \frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)a_x^* a_y^* a_y a_x \tag{4.6}$$

and the Hartree–Fock energy functional is given by

$$\mathcal{E}_{\mathrm{HF}}(\omega) = \mathrm{tr}\Big(\frac{-\hbar^2}{2}\Delta\omega\Big) + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)\omega(x,x)\omega(y,y) \\ -\frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)|\omega(x,y)|^2.$$

We will only give a sketchy proof. The conjugation of the first term of (4.6) gives

$$\begin{aligned}&\frac{\hbar^2}{2}\int \mathrm{d}x\mathrm{d}y \nabla_x\Big[a^*(u_x)+a(\overline{v}_x)\Big]\nabla_x\Big[a(u_x)+a^*(\overline{v}_x)\Big] = \frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a^*(u_x)\nabla_x a(u_x) \\ +&\frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a(\overline{v}_x)\nabla_x a^*(\overline{v}_x) + \frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a^*(u_x)\nabla_x a^*(\overline{v}_x) + \frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a(\overline{v}_x)\nabla_x a(u_x) \\ =&\frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a^*(u_x)\nabla_x a(u_x) + \frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a(\overline{v}_x)\nabla_x a^*(\overline{v}_x)\end{aligned}$$

where we used that $u(-\Delta)v = 0$ ($uv=0$ and they both commute with $-\Delta$). By bringing the terms in normal order we get

$$\begin{aligned}&\frac{\hbar^2}{2}\int \mathrm{d}x \nabla_x a^*(u_x)\nabla_x a(u_x) - \frac{\hbar^2}{2}\int \mathrm{d}x a^*(\nabla_x\overline{v}_x)a(\nabla_x\overline{v}_x) + \int \mathrm{d}x\mathrm{d}y|\nabla_x\overline{v}_x(y)|^2 \\ =&\mathrm{d}\Gamma\Big(u\Big(-\frac{\hbar^2}{2}\Delta\Big)u\Big) - \mathrm{d}\Gamma\Big(\overline{v}\Big(-\frac{\hbar^2}{2}\Delta\Big)v\Big) + \mathrm{tr}\Big(\frac{-\hbar^2}{2}\Delta\omega\Big)\end{aligned}$$

These terms give contribution to $\mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}})$ and to $\mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v)$. The conjugation of the second term of the Hamiltonian $\mathcal{H}_N$ gives 16 terms. We bring them in normal order using the anticommutation relation

$$\{a^*(\overline{v}_y), a(\overline{v}_x)\} = \omega_{\mathrm{pw}}(x,y) \qquad \text{and} \qquad \{a^*(u_y), a(\overline{v}_x)\} = 0.$$

Some of the terms construct Q_N and the two remaining parts of $\mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}})$. The remaining terms can be summarized by

$$\begin{aligned}
-\frac{1}{N}\int \mathrm{d}x\mathrm{d}y V(x-y)a^*(\overline{v}_x)a(\overline{v}_x)\omega_{\mathrm{pw}}(y,y) &= \mathrm{d}\Gamma\Big(-\overline{v}(2\pi)^3\hat{V}(0)v\Big)\\
\frac{1}{N}\int \mathrm{d}x\mathrm{d}y V(x-y)a^*(u_x)a(u_x)\omega_{\mathrm{pw}}(y,y) &= \mathrm{d}\Gamma\Big(u(2\pi)^3\hat{V}(0)u\Big)\\
\frac{1}{N}\int \mathrm{d}x\mathrm{d}y V(x-y)a^*(\overline{v}_x)a(\overline{v}_y)\omega_{\mathrm{pw}}(x,y) &= \mathrm{d}\Gamma(-\overline{v}Xv)\\
-\frac{1}{N}\int \mathrm{d}x\mathrm{d}y V(x-y)a^*(u_x)a(u_y)\omega_{\mathrm{pw}}(x,y) &= \mathrm{d}\Gamma(uXu)
\end{aligned}$$

and zero terms (because $uv = 0$). This shows (4.2).
The correlation energy is the ground state energy of the operator $R^*_{\omega_{\mathrm{pw}}}\mathcal{H}_N R_{\omega_{\mathrm{pw}}} - \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}})$. Therefore, we define the correlation Hamiltonian as

$$\mathcal{H}_{\mathrm{corr}} := \mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v) + Q_N. \tag{4.7}$$

For any normalized N-particle state $\psi \in \mathcal{F}$ in the fermionic Fock space, that is $\psi = (0,0,\ldots,0,\psi^{(N)},0,\ldots)$ we have by the variational principle and by (4.2)

$$E_N \leq \langle \psi, \mathcal{H}_N\psi\rangle = \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}}) + \langle \xi, \mathcal{H}_{\mathrm{corr}}\xi\rangle,$$

where $\xi = R^*_{\omega_{\mathrm{pw}}}\psi$. The aim is to construct an N-particle state $\psi_{\mathrm{trial}} = R_{\omega_{\mathrm{pw}}}\xi$ such that $\langle \xi, \mathcal{H}_{\mathrm{corr}}\xi\rangle$ is given by the Gell-Mann–Brueckner formula

$$\frac{\hbar\kappa_0}{2}\sum_{k\in\mathbb{Z}^3}|k|\Big[\frac{1}{\pi}\int_0^\infty \log\Big(1 + 4\pi\hat{V}(k)\kappa_0\Big(1-\lambda\arctan\frac{1}{\lambda}\Big)\Big)\mathrm{d}\lambda - \hat{V}(k)\kappa_0\pi\Big],$$

up to errors that are of smaller order as $N\to\infty$. Combining fermionic particle–hole excitations we can represent $\mathcal{H}_{\mathrm{corr}}$ in terms of almost-bosonic operators. We will see that the resulting expression will be quadratic in terms of this new operators. The trial state ξ will be chosen to minimize the corresponding bosonic energy and we will show that the expectation value of $\mathcal{H}_{\mathrm{corr}}$ in the state ξ gives the desired result.

4.2 Particle–Hole Excitations

In this section we consider the quadratic contribution Q_N of the Hamiltonian. We introduce the definition of collective particle–hole operator. Furthermore, we show that the main contribution of Q_N can be represented as a quadratic operator in terms of these particle–hole operators.

The quadratic contribution to the Hamiltonian (4.2) can be rewritten as

$$\begin{aligned}
Q_N &= Q_N^{\mathrm{B}} + \frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3}\mathrm{d}x\mathrm{d}y V(x-y)\Big(\mathcal{E}_1(x,y) + \Big[\mathcal{E}_2(x,y) + \mathrm{h.c.}\Big]\Big),\\
Q_N^{\mathrm{B}} &= \frac{1}{2N}\sum_{k\in\mathbb{Z}^3}\hat{V}(k)\int_{\mathbb{T}^3\times\mathbb{T}^3}\mathrm{d}x\mathrm{d}y\Big(2a^*(u_x)e^{ikx}a^*(\overline{v}_x)a(\overline{v}_y)e^{-iky}a(u_y)\\
&\qquad + \Big[a^*(u_x)e^{ikx}a^*(\overline{v}_x)a^*(u_y)e^{-iky}a(\overline{v}_y) + \mathrm{h.c.}\Big]\Big).
\end{aligned} \tag{4.8}$$

The term Q_N^{B} is the main contribution to Q_N. We want to represent Q_N^{B} as a quadratic Hamiltonian in terms of almost-bosonic operators. To do so, we need to introduce the (unnormalized) particle–hole operator

$$\tilde{b}_k^* := \int_{\mathbb{T}^3} \mathrm{d}x a^*(u_x) e^{ikx} a^*(\overline{v}_x) \ .$$

In momentum space we can write the creation operators as

$$a^*(u_x) = \sum_{p \in B_{\mathrm{F}}^c} e^{ipx} a_p^* \quad \text{and} \quad a^*(\overline{v}_x) = \sum_{h \in B_{\mathrm{F}}} e^{-ihx} a_h^*.$$

Then the operator b_k^* in momentum representation is given by

$$\begin{aligned} \tilde{b}_k^* &= \int a^*(u_x) e^{ikx} a^*(\overline{v}_x) \mathrm{d}x = \int \sum_{p \in B_{\mathrm{F}}^c} e^{ipx} a_p^* e^{ikx} \sum_{h \in B_{\mathrm{F}}} e^{-ihx} a_h^* \mathrm{d}x \\ &= \sum_{\substack{p \in B_{\mathrm{F}}^c \\ h \in B_{\mathrm{F}}}} a_p^* a_h^* \int e^{ix(p-h+k)} \mathrm{d}x = \sum_{\substack{p \in B_{\mathrm{F}}^c \\ h \in B_{\mathrm{F}}}} a_p^* a_h^* \delta_{p-h,k} \ . \end{aligned} \tag{4.9}$$

This operator creates a particle–hole pair of momentum k, delocalized over the whole Fermi surface. The operator Q_N^{B} can be rewritten as

$$Q_N^{\mathrm{B}} = \frac{1}{2N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \Big(2\tilde{b}_k^* \tilde{b}_k + \tilde{b}_k^* \tilde{b}_{-k}^* + \tilde{b}_{-k} \tilde{b}_k \Big).$$

Recall that we assume that our potential $\hat{V}$ is supported in a ball of radius N^μ. Thus, we only need to sum over momenta k with $|k| \leq N^\mu$. We define

$$\Gamma^{\mathrm{nor}} \subset \mathbb{Z}^3 \tag{4.10}$$

as the set of all $k \in \mathbb{Z}^3 \cap B_{N^\mu}(0)$ with $k_3 > 0$ (We use the notation k_i for the i-th component of the vector k) and additionally half of the k-vectors with $k_3 = 0$, such that for every $k \in \Gamma^{\mathrm{nor}}$ we have $-k \notin \Gamma^{\mathrm{nor}}$. So we can group together k and $-k$ modes and Q_N^{B} can be rewritten as

$$Q_N^{\mathrm{B}} = \frac{1}{2N} \sum_{k \in \Gamma^{\mathrm{nor}}} \hat{V}(k) \Big(2\tilde{b}_k^* \tilde{b}_k + \tilde{b}_k^* \tilde{b}_{-k}^* + \tilde{b}_{-k} \tilde{b}_k + 2\tilde{b}_{-k}^* \tilde{b}_{-k} + \tilde{b}_{-k}^* \tilde{b}_k^* + \tilde{b}_k \tilde{b}_{-k} \Big). \tag{4.11}$$

We shall show that, whenever acting on vectors of $\mathcal{F}$ with only a few particles, the operators $\tilde{b}_k$ behave as approximate bosonic operators. The Pauli principle is relaxed by summing over a large number of momenta of which typically only a few are occupied. The problem is that $\mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v)$ in (4.2) can not be written as a quadratic operator in terms of $\tilde{b}_k$ and $\tilde{b}_k^*$. To avoid this issue we shall split the operators $\tilde{b}_k$ and $\tilde{b}_k^*$ into partially localized particle–hole operators $\tilde{b}_{\alpha,k}$ and $\tilde{b}_{\alpha,k}^*$ involving only modes of one patch (indexed by α) of a decomposition of the Fermi surface. We then can linearize the kinetic energy around the centers of the patches. The difficulty is to localize the particle–hole operators sufficiently to control the linearization of the kinetic energy but also to keep it sufficiently delocalized such that the operators involve many modes and to become approximately bosonic operators by relaxing the Pauli principle.

4.2.1 Patch Decomposition of the Fermi Sphere

The next step is to decompose the Fermi sphere into patches of equal area such that the diameter is bounded. Neighboring patches should be separated by a positive distance (called the "corridors") such that the the area of the corridors is of small order.

We divide the Fermi sphere $k_F\mathbb{S}^2$ into M diameter-bounded equal-area patches, where

$$M = M(N) := N^{1/3+\epsilon} \text{ for an } 0 < \epsilon < 1/3 - 2\mu$$

rounded to the nearest even integer. First, we decompose the unit sphere $\mathbb{S}^2$ as

$$\mathbb{S}^2 = \left(\bigcup_{\alpha=1}^{M} p_\alpha \right) \cup p_{\text{corri}} \ ,$$

where p_α are pairwise disjoint sets, defined below, separated by p_{corri}. The corridor p_{corri} has small surface measure, $\sigma(p_{\text{corri}}) = \mathcal{O}(M^{1/2}N^{-1/3+\mu}) \to 0$ as $N \to \infty$. The patches p_α admit two important properties. First, their area is of order $1/M$. Second, due to the bounded diameter they do not degenerate into very long, thin shapes as M grows.

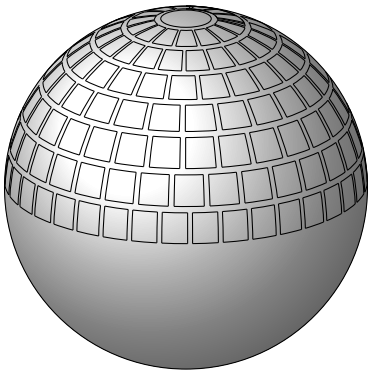

Figure 4.2: Decomposition of the norther half unit sphere into diameter-bounded patches of equal-area

We use standard spherical coordinates for the decomposition. A point on the sphere $\hat{\omega} \in \mathbb{S}^2$ is described by θ, the inclination angle measured between $\hat{\omega}$ and $e_3 = (0, 0, 1)$, and by ϕ, the azimuth angle measured between $e_1 = (1, 0, 0)$ and the projection of $\hat{\omega}$ onto the plane orthogonal to e_3. We write $\hat{\omega}(\theta, \phi)$ to characterize a point on the unit sphere in terms of its inclination and azimuth angle.

For the construction, we first need to place a spherical cap centered at e_3, with opening angle $\Delta\theta_0 := D/\sqrt{M}$, with $D \in \mathbb{R}$ chosen such that the area of the spherical cap equals $4\pi/M$. The remaining part of the half sphere is decomposed into $\sqrt{M}/2$ (rounded to the next integer) collars. The i-th collar consists of all $\hat{\omega}(\theta, \phi)$ with $\theta \in [\theta_i - \Delta\theta_i, \theta_i + \Delta\theta_i)$ and arbitrary azimuth ϕ. We have $\Delta\theta_i \sim 1/\sqrt{M}$; the proportionality constant is chosen such that the number of collars is an integer. The circumference of the circle in the i-th collar $\{\hat{\omega}(\theta_i, \phi) : \phi \in [0, 2\pi)\}$ is $2\pi \sin(\theta_i)$. Thus, we split the i-th collar into $\frac{\pi}{2}\sqrt{M}\sin(\theta_i)$

patches, rounded to the next integer. The j-th patch in the i-th collar covers an azimuth angle $\phi \in [\phi_{i,j} - \Delta\phi_{i,j}, \phi_{i,j} + \Delta\phi_{i,j})$, where

$$\Delta\phi_{i,j} \sim \frac{1}{\sin(\theta_i)\sqrt{M}}.$$

The proportionality constants are chosen in a way to guarantees that all patches have area of order $4\pi/M$. We still need to introduce the positive distance between neighboring patches. We define $\Delta\tilde{\theta}_i := \Delta\theta_i - \tilde{D}N^{\mu-1/3}$ and $\Delta\tilde{\phi}_{i,j} := \Delta\phi_{i,j} - \tilde{D}N^{\mu-1/3}/\sin(\theta_i)$, with $\tilde{D} > 0$ to be fixed below. We set p_1 as the spherical cap centered at e_3 with opening angle $\Delta\tilde{\theta}_0$ and the other $M/2 - 1$ patches as

$$p_{i,j} := \Big\{\tilde{\omega}(\theta,\phi) : \theta \in [\theta_i - \Delta\tilde{\theta}_i, \theta_i + \Delta\tilde{\theta}_i) \text{ and } \phi \in [\phi_{i,j} - \Delta\tilde{\phi}_{i,j}, \phi_{i,j} + \Delta\tilde{\phi}_{i,j})\Big\}.$$

The constant $\tilde{D}$ is chosen such that there are corridors of width at least $2N^\mu$ between adjacent patches, when scaling the patches up to the Fermi sphere. Reflection at the origin, $k \to -k$, expands the construction to the southern half sphere. We switch from enumeration by i and j to enumeration with a single index $\alpha \in \{1, \dots, M\}$. The patches p_α have the following properties, derived by the construction:

(i) The area of every patch is

$$\sigma(p_\alpha) = \frac{4\pi}{M} + \mathcal{O}(N^{-1/3+\mu}M^{-1/2}).$$

(ii) The family of decompositions is diameter-bounded, i.e, there exists a constant C_0 independent of N and M such that the diameter of every patch is bounded by $C_0/\sqrt{M}$.

(iii) Point reflection at the origin maps p_α to $-p_\alpha = p_{\alpha+\frac{M}{2}}$ for all $\alpha = 1, \dots, \frac{M}{2}$.

We need the decomposition of the Fermi surface $k_\mathrm{F}\mathbb{S}^2$. To reach this, we scale our patches with the factor k_F. We set

$$P_\alpha := k_\mathrm{F} p_\alpha$$

for all $\alpha = 1, \dots M$. The properties above are adapted and we obtain the following properties for the patches P_α:

(i) The area of every patch is

$$\sigma(P_\alpha) = \frac{4\pi}{M}k_\mathrm{F}^2 + \mathcal{O}(N^{1/3+\mu}M^{-1/2}).$$

(ii) There exists a constant C_1 independent of N and M such that, for the decomposition in M patches, the diameter of every patch is bounded by $C_1 N^{1/3}/\sqrt{M}$.

The aim is to split the operator $\tilde{b}_k$ and $\tilde{b}_k^*$ into partially localized particle–hole operators. Recall the definition of the particle–hole operator (4.9) and of Q_N^B (4.11) and note that the potential $\hat{V}$ is zero outside a ball of radius N^μ. We conclude that we only need to consider particle and hole modes a distance at most N^μ from the Fermi sphere. Therefore,

we want to introduce a "fattening" of the patch decomposition, where the thickness of the shell is given by N^μ. First, we define the fattened Fermi surface as

$$\partial B_{\mathrm{F}}^{N^\mu} := \Big\{ q \in \mathbb{Z}^3 : k_{\mathrm{F}} - N^\mu \leq |q| \leq k_{\mathrm{F}} + N^\mu \Big\}.$$

Let us introduce the cones $C_\alpha := \cup_{r\in(0,\infty)} r p_\alpha$ and set

$$B_\alpha := \partial B_{\mathrm{F}}^{N^\mu} \cap C_\alpha$$

for the "fattening" of the patch P_α. Now we can decompose $\partial B_{\mathrm{F}}^{N^\mu}$ as

$$\partial B_{\mathrm{F}}^{N^\mu} = \left(\bigcup_{\alpha=1}^{M} B_\alpha \right) \cup B_{\mathrm{corri}}$$

where the set B_{corri} consist of all the remaining modes in the similarly fattened corridors. To every patch B_α we assign a vector $\omega_\alpha \in B_\alpha$ as the center of P_α on the Fermi surface.

4.2.2 Localization on the Fermi Surface

We are now ready to localize the particle–hole operators on the Fermi ball. The new operators should only affect modes in a single patch B_α.

Recall that

$$\tilde{b}_k^* = \sum_{\substack{p\in B_{\mathrm{F}}^c \\ h\in B_{\mathrm{F}}}} a_p^* a_h^* \delta_{p-h,k}. \tag{4.12}$$

As already mentioned we only need to consider $|k| \leq N^\mu$. This means the sum runs only over p and h a distance at most N^μ from the Fermi sphere $k_{\mathrm{F}}\mathbb{S}^2$. Hence,

$$\tilde{b}_k^* = \sum_{\substack{p\in B_{\mathrm{F}}^c \cap \partial B_{\mathrm{F}}^{N^\mu} \\ h\in B_{\mathrm{F}} \cap \partial B_{\mathrm{F}}^{N^\mu}}} a_p^* a_h^* \delta_{p-h,k}. \tag{4.13}$$

We decompose the sum on the r.h.s. into contributions associated to different patches. If $k \cdot \omega_\alpha < 0$ no particle–hole pair $(p,\, h)$ in the patch B_α satisfy $p - h = k$. The reason is that k points approximately form outside to inside of the Fermi ball and no excitation is possible. Additionally, if $k \cdot \omega_\alpha$ is positive but small, we find only a few particle–hole pairs (p, h) with $p - h = k$ in the patch B_α. This motivates the following definition of the index set

$$\mathcal{I}_k^+ := \{\alpha = 1, \ldots, M : \hat{\omega}_\alpha \cdot \hat{k} \geq N^{-\delta}\}$$

for $0 < \delta < 1/6 - \varepsilon/2 - \mu$ and for $\hat{k} := k/|k|$. We can now rewrite the particle–hole operator as

$$\tilde{b}_k^* = \sum_{\alpha\in\mathcal{I}_k^+} \tilde{b}_{\alpha,k}^* + \mathfrak{r}_k^* \,, \tag{4.14}$$

where

$$\tilde{b}_{\alpha,k}^* := \sum_{\substack{p\in B_{\mathrm{F}}^c \cap B_\alpha \\ h\in B_{\mathrm{F}} \cap B_\alpha}} a_p^* a_h^* \delta_{p-h,k}.$$

The operator $\mathfrak{r}_k^*$ contains all particle–hole pairs that are not included in $\sum_{\alpha\in\mathcal{I}_k^+}\tilde{b}_{\alpha,k}^*$. This happens if an index α is not included in $\mathcal{I}_k^+$ or if one or both momenta of a pair $(p,\, h)$ belong to the corridor between the patches. Note that it is not possible for a particle mode p and a hole mode h, with $p-h=k$ (with $|k|\leq N^\mu$), to be in different patches, since we chose the decomposition in such a way that the distance between two distinct patches is larger than N^μ.

4.2.3 Normalization of Particle–Hole Pair Operator

In order to have approximately bosonic operators, we need to normalize the pair operators. The normalized operators are defined by

$$b_{\alpha,k}^* := \frac{1}{n_{\alpha,k}}\tilde{b}_{\alpha,k}^*, \quad n_{\alpha,k} := \|\tilde{b}_{\alpha,k}^*\Omega\|.$$

These operators are called the pair creation operator (creates excitations with momentum k) and their adjoints are called pair annihilation operators (annihilates excitations with momentum k). The normalization constant can be calculated as follows

$$\begin{aligned}
\|\tilde{b}_{\alpha,k}^*\Omega\|^2 &= \langle\Omega, \left[\sum_{\substack{p_1\in B_{\mathrm{F}}^c\cap B_\alpha\\ h_1\in B_{\mathrm{F}}\cap B_\alpha}} a_{p_1}^* a_{h_1}^* \delta_{p_1-h_1,k}\right]^* \left[\sum_{\substack{p_2\in B_{\mathrm{F}}^c\cap B_\alpha\\ h_2\in B_{\mathrm{F}}\cap B_\alpha}} a_{p_2}^* a_{h_2}^* \delta_{p_2-h_2,k}\right]\Omega\rangle \\
&= \langle\Omega, \sum_{\substack{p_1,p_2\in B_{\mathrm{F}}^c\cap B_\alpha\\ h_1,h_2\in B_{\mathrm{F}}\cap B_\alpha}} a_{p_1} a_{p_2}^* a_{h_1} a_{h_2}^* \delta_{p_1-h_1,k}\delta_{p_2-h_2,k}\Omega\rangle \\
&= \langle\Omega, \sum_{\substack{p_1,p_2\in B_{\mathrm{F}}^c\cap B_\alpha\\ h_1,h_2\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p_1,p_2}\delta_{h_1,h_2}\delta_{p_1-h_1,k}\delta_{p_2-h_2,k}\Omega\rangle = \sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha\\ h\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p-h,k}.
\end{aligned}$$

This shows that $n_{\alpha,k}^2$ is the number of particle–hole pairs with momentum $k=p-h$ that lie in the patch B_α. We define $v_\alpha(k)\geq 0$ by setting

$$n_{\alpha,k}^2 =: k_{\mathrm{F}}^2|k|v_\alpha(k)^2. \tag{4.15}$$

The next proposition gives an estimate on the normalization constants.

Proposition 4.1. *Let $k\in\mathbb{Z}^3\setminus\{0\}$, $M=N^{1/3+\epsilon}$ for an $0<\epsilon<1/3-2\mu$. Then, for $0<\delta<1/6-\epsilon/2-\mu$ and for all $\alpha\in\mathcal{I}_k^+$, we have*

$$v_\alpha(k)^2 = \sigma(p_\alpha)|\hat{k}\cdot\hat{\omega}_\alpha|\left(1+\mathcal{O}(\sqrt{M}N^{-1/3+\delta+\mu})\right),$$

where $\sigma(p_\alpha)=\frac{4\pi}{M}+\mathcal{O}(N^{-1/3+\mu}M^{-1/2})$ is the surface area of the patch p_α on the unit sphere.

Since $\hat{\omega}_\alpha\cdot\hat{k}\geq N^{-\delta}$, imposed through the index set $\mathcal{I}_k^+$, it follows that there exists a constant C such that

$$n_{\alpha,k}\geq C\mathfrak{n}, \quad \text{where} \quad \mathfrak{n}(N,M) := \frac{N^{1/3-\delta/2}}{\sqrt{M}}. \tag{4.16}$$

Proof. We are going to prove the following equivalent statement: Assuming that $0 < \delta < \frac{1}{6} - \frac{\epsilon}{2} - \mu$ and $\alpha \in \mathcal{I}_k^+$ the number of particle–hole pairs with momentum k in the patch B_α is

$$n_{\alpha,k}^2 = |\hat{k} \cdot \hat{\omega}_\alpha| k_{\mathrm{F}}^2 \sigma(p_\alpha) |k| \Big(1 + \mathcal{O}\Big(\sqrt{M} N^{-\frac{1}{3}+\delta+\mu}\Big)\Big). \tag{4.17}$$

Let $k = (k_1, k_2, k_3)$, and consider a patch P_α on the Fermi sphere. Due to symmetry, we can assume that k_1, k_2 and k_3 are all non-negative, and without loss of generality we assume $k_3 \neq 0$ (if $k_3 = 0$ we would project onto another coordinate plane). Let P_α^k be the projection of P_α along k onto $\mathbb{R}^2 \times \{0\}$, i.e. the plane spanned by e_1 and e_2.

The first task is to calculate the Lebesgue measure of P_α^k, i.e. $\mu(P_\alpha^k)$. Consider the lines $\{k_{\mathrm{F}} \hat{\omega}(\theta, \phi) + tk : t \in \mathbb{R}\}$. Their intersection with $\mathbb{R}^2 \times \{0\}$ is at $t = -k_{\mathrm{F}} \hat{\omega}(\theta, \phi)_3 / k_3$, so

$$P_\alpha^k := \Big\{ (x(\theta,\phi), y(\theta,\phi), 0) = k_{\mathrm{F}} \hat{\omega}(\theta,\phi) - \frac{k_{\mathrm{F}}}{k_3} \hat{\omega}(\theta,\phi)_3 k : \hat{\omega}(\theta,\phi) \in p_\alpha \Big\} \subset \mathbb{R}^2 \times \{0\}.$$

Writing $\Phi(\theta, \phi) = (x(\theta, \phi), y(\theta, \phi))$, we find that P_α^k has two-dimensional Lebesgue measure

$$\mu\Big(P_\alpha^k\Big) = \int_{P_\alpha^k} \mathrm{d}x \mathrm{d}y = \int_{p_\alpha} |\mathrm{det} D\Phi(\theta,\phi)| \mathrm{d}\theta \mathrm{d}\phi.$$

Using $\hat{\omega}(\theta, \phi) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ we can calculate the Jacobi determinant

$$|\mathrm{det} D\Phi(\theta,\phi)| = k_{\mathrm{F}}^2 \frac{|\sin\theta|}{k_3} |k_1 \sin\theta\cos\phi + k_2 \sin\theta\sin\phi + k_3\cos\theta| = k_{\mathrm{F}}^2 \frac{|\sin\theta|}{k_3} |k \cdot \hat{\omega}(\theta,\phi)|.$$

Since the patch is diameter-bounded by $C/\sqrt{M}$ and $|k|$ is bounded by N^μ we have $|k \cdot \omega(\theta,\phi)| = |k \cdot \hat{\omega}_\alpha| + \mathcal{O}(M^{-1/2} N^\mu)$. Additionally, we use $|\hat{k} \cdot \hat{\omega}_\alpha| \geq N^{-\delta}$ to convert the additive error into a multiplicative error. We get

$$\mu(P_\alpha^k) = \frac{k_{\mathrm{F}}^2}{k_3} \int_{p_\alpha} |k \cdot \hat{\omega}(\theta,\phi)| |\sin\theta| \mathrm{d}\theta \mathrm{d}\phi = \frac{k_{\mathrm{F}}^2}{k_3} |k \cdot \hat{\omega}_\alpha| \Big(1 + \mathcal{O}\Big(M^{-1/2} N^{\mu+\delta}\Big)\Big) \sigma(p_\alpha). \tag{4.18}$$

We now determine the distance between neighboring lattice points along every line

$$L_n := \{n + tk : t \in \mathbb{R}\} \qquad \text{where } n \in \mathbb{Z}^3.$$

Let $p := \gcd(k_1, k_2, k_3)$ be the greatest common divisor of the components of k. The distance between neighboring lattice points on each line L_n is $|k|/p$. Given a line L_n intersecting P_α, let $h \in L_n \cap B_{\mathrm{F}}$ be the lattice point closest to P_α. Then on the line segment $\{h + tk : t \in (0, 1]\}$ there are p lattice points, by shifting along the line (take $t = 1/p, 2/p, \ldots, (p-1)/p, 1$). These correspond to p particle–hole pairs contributing to $n_{\alpha,k}^2$. We conclude that $n_{\alpha,k}^2$ is to leading order the number of lattice lines L_n intersecting P_α^k multiplied with $\gcd(k_1, k_2, k_3)$.
We need to determine how many lattice lines run through P_α^k. For this purpose set $L := \cup_{n \in \mathbb{Z}^3} L_n$. The intersection of L_n with $\mathbb{R}^2 \times \{0\}$ is at $t = -n_3/k_3$. Thus,

$$L \cap (\mathbb{R}^2 \times \{0\}) = \Big\{ \Big(n_1 - n_3 \frac{k_1}{k_3}, n_2 - n_3 \frac{k_2}{k_3}, 0\Big) : n \in \mathbb{Z}^3 \Big\}.$$

This can be seen as the two-dimensional square lattice $\mathbb{Z}^2$ (the translates of the unit square indexed by n_1 and n_2) and a point pattern repeated in every lattice translation of the unit square. As soon as n_3k_1/k_3 and n_3k_2/k_3 simultaneously become integer, we start repeating the point pattern in another translate of the unit square. So the number of points in the unit square is the smallest integer n_3 such that both n_3k_1/k_3 and n_3k_2/k_3 are integer. We claim that this is when $n_3 = k_3/p$.
To prove this claim, consider the fraction k_1/k_3. Obviously, n_3k_1/k_3 is an integer if and only if n_3 is a multiple of $k_3/\gcd(k_1, k_3)$. Similarly, n_3k_2/k_3 is integer if and only if n_3 is a multiple of $k_3/\gcd(k_2, k_3)$. So the number of points in the unit square is given by their least common multiple,

$$\#\text{points in unit square} = \operatorname{lcm}\Big(\frac{k_3}{\gcd(k_1,k_3)}, \frac{k_3}{\gcd(k_2,k_3)}\Big).$$

From the standard identity $\gcd(a, b) \cdot \operatorname{lcm}(a, b) = |ab|$ for all $a, b \in \mathbb{Z}$ we get

$$\operatorname{lcm}\Big(\frac{k_3}{\gcd(k_1,k_3)}, \frac{k_3}{\gcd(k_2,k_3)}\Big) = \frac{k_3^2}{\gcd(k_1,k_3)\gcd(k_2,k_3)\gcd\left(\frac{k_3}{\gcd(k_1,k_3)}, \frac{k_3}{\gcd(k_2,k_3)}\right)}.$$

Using twice the fact that $m \cdot \gcd(a, b) = \gcd(ma, mb)$ for all $m \in \mathbb{N}$ (once with $m = \gcd(k_1, k_3)$ and once with $m = \gcd(k_2, k_3)$), the same fact in inverse direction with $m = k_3$ and $\gcd(a, b, c) = \gcd(\gcd(b, c), \gcd(a, c))$ yields

$$= \frac{k_3^2}{\gcd(k_3\gcd(k_2,k_3), k_3\gcd(k_1,k_3))} = \frac{k_3}{\gcd(\gcd(k_2,k_3), \gcd(k_1,k_3))} = \frac{k_3}{\gcd(k_1,k_2,k_3)}.$$

In extension of Gauss' argument, the number of lines intersecting P_α^k is equal to the Lebesgue measure of P_α^k times the number of intersection points per unit square. We conclude that

$$n_{\alpha,k}^2 = \mu\Big(P_\alpha^k\Big)k_3 + \mathfrak{e}_{\alpha,k}. \tag{4.19}$$

The error term $\mathfrak{e}_{\alpha,k}$ is proportional to the circumference of P_α^k times the number of lines per unit square. Consider a patch that is not a spherical cap (the estimate for the two spherical caps works analogously). Its circumference consists of four pieces. The first piece is parametrized by $\gamma(\phi) := \Phi(\theta_\alpha + \Delta\theta_\alpha, \phi)$, and has length

$$\int_{\phi_\alpha-\Delta\phi_\alpha}^{\phi+\Delta\phi_\alpha} |\dot\gamma(\phi)|\mathrm{d}\phi = 2\Delta\phi_\alpha k_\mathrm{F}|\sin(\theta_\alpha + \Delta\theta_\alpha)| = \mathcal{O}\Big(\frac{k_\mathrm{F}}{\sqrt{M}}\Big).$$

The second piece, parametrized by $\phi \to \Phi(\theta_\alpha - \Delta\theta, \phi)$, is of the same order. The third piece is parametrized by $\tilde\gamma(\theta) := \Phi(\theta, \phi_\alpha + \Delta\phi_\alpha)$. We estimate

$$\begin{aligned}
&|\dot{\tilde\gamma}(\theta)|^2 \\
&= \frac{k_\mathrm{F}^2}{k_3^2}\Big|k_3^2\cos^2\theta + (k_1^2+k_2^2)\sin^2\theta + 2k_3\cos\theta\sin\theta\Big[k_1\cos(\phi_\alpha+\Delta\phi_\alpha) + k_2\sin(\phi_\alpha+\Delta\phi_\alpha)\Big]\Big| \\
&\le 2\frac{k_\mathrm{F}^2}{k_3^2}|k|^2
\end{aligned}$$

Integrating and recalling that $\Delta\theta_\alpha = \mathcal{O}(M^{-1/2})$, the length of this piece is at most of order $k_{\mathrm{F}}/k_3 N^\mu M^{-1/2}$. The fourth piece has length of the same order as the third piece. We conclude that $|\mathfrak{e}_{\alpha,k}| = \mathcal{O}(k_{\mathrm{F}} M^{-1/2} N^\mu)$. We have

$$\begin{aligned}
n_{\alpha,k}^2 &= \mu(P_\alpha^k) k_3 + \mathfrak{e}_{\alpha,k} \\
&= \frac{k_{\mathrm{F}}^2}{k_3} |k \cdot \hat{\omega}_\alpha| \Big(1 + \mathcal{O}\Big(M^{-1/2} N^{\delta+\mu}\Big)\Big) \sigma(p_\alpha) \cdot k_3 + \mathcal{O}\Big(k_{\mathrm{F}} M^{-1/2} N^\mu\Big) \\
&= k_{\mathrm{F}}^2 |k \cdot \hat{\omega}_\alpha| \Big(1 + \mathcal{O}\Big(M^{-1/2} N^{\delta+\mu}\Big)\Big) \sigma(p_\alpha) + \mathcal{O}\Big(k_{\mathrm{F}} M^{-1/2} N^\mu\Big) \\
&= k_{\mathrm{F}}^2 |k \cdot \hat{\omega}_a| \sigma(p_\alpha) \Big(1 + \mathcal{O}\Big(M^{-1/2} N^{\delta+\mu}\Big) + \mathcal{O}\Big(k_{\mathrm{F}}^{-1} N^\delta M^{1/2} N^\mu\Big)\Big) \\
&= k_{\mathrm{F}}^2 |k \cdot \hat{\omega}_a| \sigma(p_\alpha) \Big(1 + \mathcal{O}\Big(k_{\mathrm{F}}^{-1} N^\delta M^{1/2} N^\mu\Big)\Big)
\end{aligned}$$

where we combined (4.19) with (4.18), and used $|\hat{k} \cdot \hat{\omega}_\alpha| \geq N^{-\delta}$ to convert the additive error into a multiplicative error (the second error term is the dominating one). This shows (4.17). □

Chapter 5

Construction of the Trial State

The aim of this chapter is to define a suitable trial state which generates the desired upper bound for the ground state energy. We will see that we can obtain the trial state by an action of an approximate Bogoliubov transformation. At the end we will give some useful properties of this transformation.

5.1 Particle–Hole Creation via Almost-Bosonic Operators

First we will show that the particle–hole operators $b_{\alpha,k}$, constructed in the previous chapter, behave approximately as bosonic operators.

For $k \in \Gamma^{\mathrm{nor}}$, let

$$\mathcal{I}_k^- := \mathcal{I}_{-k}^+ = \{\alpha = 1, \dots, M : \hat{\omega}_\alpha \cdot \hat{k} \leq -N^{-\delta}\}.$$

We consider the union of the sets $\mathcal{I}_k^+$ and $\mathcal{I}_k^-$ and denote it by $\mathcal{I}_k = \mathcal{I}_k^+ \cup \mathcal{I}_k^-$. Each $\alpha \in \{1, \dots, M\}$ is at most part of only one $\mathcal{I}_k^+$ or $\mathcal{I}_{-k}^+$. Thus, we can combine the two operators $b_{\alpha,k}^*$ and $b_{\alpha,-k}^*$ and only considering $k \in \Gamma^{\mathrm{nor}}$. We define

$$c_\alpha^*(k) := \begin{cases} b_{\alpha,k}^* & \text{for } \alpha \in \mathcal{I}_k^+ \\ b_{\alpha,-k}^* & \text{for } \alpha \in \mathcal{I}_k^- \end{cases}. \tag{5.1}$$

The following lemma shows that the operators $c_\alpha^*(k)$ and $c_\alpha(k)$ behave as almost bosonic operators when acting on states with only a few particles.

Lemma 5.1 (Approximate CCR)**.** *Let $k, l \in \Gamma^{\mathrm{nor}}$. Let $\alpha \in \mathcal{I}_k$ and $\beta \in \mathcal{I}_l$. Then*

$$\begin{aligned} &[c_\alpha(k), c_\beta(l)] = 0 = [c_\alpha^*(k), c_\beta^*] \ , \\ &[c_\alpha(k), c_\beta^*(l)] = \delta_{\alpha,\beta}(\delta_{k,l} + \mathcal{E}_\alpha(k,l)). \end{aligned} \tag{5.2}$$

The operator $\mathcal{E}_\alpha(k,l)$ commutes with $\mathcal{N}$, and satisfies the bound

$$\|\mathcal{E}_\alpha(k,l)\psi\| \leq \frac{2}{n_{\alpha,k} n_{\alpha,l}} \|\mathcal{N}\psi\| \ , \quad \forall \psi \in \mathcal{F} \tag{5.3}$$

The same estimate holds for $\mathcal{E}_\alpha^*(k,l) = \mathcal{E}_\alpha(l,k)$.

The Inequality (5.3) shows that the bosonic behaviour holds for states with few particles. Otherwise the l.h.s. would be large.

Proof. The two identities on the first line of (5.2) follow from the facts that the annihilation operators commute with each other as well as the creation operators.
To prove the second line we need to consider different cases.

First case: $\alpha \in \mathcal{I}_k^+$ and $\beta \in \mathcal{I}_k^+$.
We have

$$[c_\alpha(k), c_\beta^*(l)] = [b_{\alpha,k}, b_{\beta,l}^*].$$

If the operators b and b^* belong to different patches, they will commute. This explains the $\delta_{\alpha,\beta}$-factor. From now on we can assume that α is equal to β. By the CAR,

$$[a_{h_1}a_{p_1}, a_{p_2}^*, a_{h_2}^*] = \delta_{h_1,h_2}\delta_{p_1,p_2} - a_{p_2^*}a_{p_1}\delta_{h_1,h_2} - a_{h_2}^*a_{h_1}\delta_{p_1,p_2}.$$

The first term produces the following contribution to the commutator

$$\begin{aligned} &n_{\alpha,k}^{-1}n_{\alpha,l}^{-1} \sum_{\substack{p_1\in B_{\mathrm{F}}^c\cap B_\alpha \\ h_1\in B_{\mathrm{F}}\cap B_\alpha}} \sum_{\substack{p_2\in B_{\mathrm{F}}^c\cap B_\alpha \\ h_2\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{h_1,h_2}\delta_{p_1,p_2}\delta_{p_1-h_1,k}\delta_{p_2-h_2,l} \\ &= n_{\alpha,k}^{-1}n_{\alpha,l}^{-1} \sum_{\substack{p_1\in B_{\mathrm{F}}^c\cap B_\alpha \\ h_1\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p_1-h_1,k}\delta_{p_1-h_1,l} = n_{\alpha,k}^{-2}\delta_{k,l} \sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p-h,k} = \delta_{k,l}. \end{aligned}$$

The last two terms give the error term

$$\begin{aligned} &- \sum_{\substack{h_1,h_2\in B_{\mathrm{F}}\cap B_\alpha \\ p\in B_{\mathrm{F}}^c\cap B_\alpha}} \frac{\delta_{p-h_1,k}\delta_{p-h_2,l}}{n_{\alpha,k}n_{\alpha,l}} a_{h_2}^*a_{h_1} - \sum_{\substack{p_1,p_2\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} \frac{\delta_{p_1-h,k}\delta_{p_2-h,l}}{n_{\alpha,k}n_{\alpha,l}} a_{p_2}^*a_{p_1} \\ &\qquad =: \mathcal{E}_1(\alpha,k,l) + \mathcal{E}_2(\alpha,k,l) =: \mathcal{E}(\alpha,k,l) \end{aligned} \tag{5.4}$$

The error in the statement is defined as $\mathcal{E}_\alpha(k,l) := \mathcal{E}(\alpha,k,l)$. First we will estimate the second term in the l.h.s.. We will use the operators $\omega^{(\alpha)} := \sum_{h\in B_{\mathrm{F}}\cap B_\alpha} |f_h\rangle\langle f_h|$ and $u^{(\alpha)} := \sum_{p\in B_{\mathrm{F}}^c\cap B_\alpha} |f_p\rangle\langle f_p|$. We have

$$\begin{aligned} \mathrm{d}\Gamma\Big(u^{(\alpha)}e^{ilx}\omega^{(\alpha)}e^{-ikx}u^{(\alpha)}\Big) &= \sum_{p_1,p_2\in B_{\mathrm{F}}^c\cap B_\alpha} a_{p_1}^*a_{p_2}\langle f_{p_2}, e^{ilx}\Big[\sum_{h\in B_{\mathrm{F}}\cap B_\alpha} |f_h\rangle\langle f_h|\Big]e^{-ikx}|f_{p_1}\rangle \\ &= \sum_{\substack{p_1,p_2\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} a_{p_1}^*a_{p_2}\delta_{p_2-h,l}\delta_{p_1-h,k}. \end{aligned}$$

For any bounded one-particle operator we have by Lemma 2.6 the bound $\|\mathrm{d}\Gamma(A)\psi\| \leq \|A\|_{\mathrm{op}}\|\mathcal{N}\psi\|$ for all $\psi \in \mathcal{N}$. Therefore,

$$\|\mathcal{E}_2(\alpha,k,l)\psi\| = \left\|\frac{1}{n_{\alpha,k}n_{\alpha,l}}\mathrm{d}\Gamma\Big(u^{(\alpha)}e^{ilx}\omega^{(\alpha)}e^{-ikx}u^{(\alpha)}\Big)\right\| \leq \frac{1}{n_{\alpha,k}n_{\alpha,l}}\|\mathcal{N}\psi\|$$

since $\|u^{(\alpha)}e^{ilx}\omega^{(\alpha)}e^{-ikx}u^{(\alpha)}\|_{\mathrm{op}} \leq 1$. The first term on the l.h.s. can be estimated similarly

$$\begin{aligned}\mathrm{d}\Gamma\Big(\omega^{(\alpha)}e^{-ilx}u^{(\alpha)}e^{ikx}\omega^{(\alpha)}\Big) &= \sum_{h_1,h_2\in B_{\mathrm{F}}\cap B_\alpha} a^*_{h_2}a_{h_1}\langle f_{h_1}, e^{-ilx}\Big[\sum_{p\in B_{\mathrm{F}}^c\cap B_\alpha}|f_p\rangle\langle f_p|\Big]e^{-ikx}|f_{h_2}\rangle \\ &= \sum_{h_1,h_2\in B_{\mathrm{F}}} a^*_{h_2}a_{h_1}\delta_{p-h_1,l}\delta_{p-h_2,k}.\end{aligned}$$

With the similar bounds as for the second term we conclude that

$$\|\mathcal{E}_1(\alpha,k,l)\psi\| \leq \frac{1}{n_{\alpha,k}n_{\alpha,l}}\|\mathcal{N}\psi\|.$$

Second case: $\alpha \in \mathcal{I}_k^-$ and $\beta \in \mathcal{I}_l^-$.
This case is treated like the first case, recalling that

$$[c_\alpha(k), c^*_\beta(l)] = [b_{\alpha,-k}, b^*_{\beta,-l}].$$

The error is defined as $\mathcal{E}_\alpha(k,l) := \mathcal{E}(\alpha,-k,-l)$, with the same bound as before.

Third case: $\alpha \in \mathcal{I}_k^+$ and $\beta \in \mathcal{I}_l^-$, and vice versa.
Again, we can assume that $\alpha = \beta$, otherwise the commutator vanishes. So we have $\alpha \in \mathcal{I}_k^+$ and $\alpha = \beta \in \mathcal{I}_l^- = \mathcal{I}_{-l}^+$. We find

$$[c_\alpha(k), c^*_\beta(l)] = [b_{\alpha,k}, b^*_{\alpha,-l}] = \delta_{k,-l} + \mathcal{E}(\alpha,k,-l).$$

For $\alpha = \beta$ we need to exclude $k = l$ since $\mathcal{I}_k^+ \cap \mathcal{I}_k^- = \emptyset$. Also $k = -l$ since $k, l \in \Gamma^{\mathrm{nor}}$. Therefore $\delta_{k,l} = 0 = \delta_{k,-l}$. Together with the error $\mathcal{E}_\alpha(k,l) := \mathcal{E}(\alpha,k,-l)$ the commutator agrees with the one of the lemma. The estimate for the error term remains the same.

We still need to show that the error term commutes with $\mathcal{N}$. For this purpose, notice that the operator $a^*_{h_2}a_{h_1}$ and $a^*_{p_2}a_{p_1}$ respectively commutes with the number of particle operator $\mathcal{N}$ because for each annihilated fermion (with momentum h_1 and p_1 respectively) a fermion is created by the operators $a^*_{h_2}$ and $a^*_{p_2}$ respectively. We conclude that the commutator of $\mathcal{N}$ and $\mathcal{E}_\alpha(k,l)$ vanishes. This completes the proof of the lemma. □

The next lemma gives bounds for the operator $c_\alpha(k)$ and $c^*_\alpha(k)$ similar to the usual bounds for bosonic creation and annihilation operators.

Lemma 5.2 (Bounds for Pair Operators)**.** *Let $k \in \Gamma^{\mathrm{nor}}$ and $\alpha \in \mathcal{I}_k$. Then,*

$$\|c_\alpha(k)\psi\| \leq \|\mathcal{N}(B_{\mathrm{F}}\cap B_\alpha)^{1/2}\psi\| \quad \forall\psi\in\mathcal{F}, \tag{5.5}$$

where $\mathcal{N}(B) := \sum_{i\in B} a_i^*a_i$ for any set of momenta $B \subset \mathbb{Z}^3$. Furthermore, for $f \in \ell^2(\mathcal{I}_k)$ and $\psi \in \mathcal{F}$, we have

$$\begin{aligned}\|\sum_{\alpha\in\mathcal{I}_k} f(\alpha)c_\alpha(k)\psi\| &\leq \Big(\sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\Big)^{1/2}\|\mathcal{N}^{1/2}\psi\|, \\ \|\sum_{\alpha\in\mathcal{I}_k} f(\alpha)c^*_\alpha(k)\psi\| &\leq \Big(\sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\Big)^{1/2}\|(\mathcal{N}+1)^{1/2}\psi\|.\end{aligned} \tag{5.6}$$

Proof. Using $\|a_q\|_{\mathrm{op}} = 1$, we have

$$\begin{aligned}\|b_{\alpha,k}\psi\| &\leq \frac{1}{n_{\alpha,k}} \sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p-h,k}\|a_p a_h\psi\| \leq \frac{1}{n_{\alpha,k}} \sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p-h,k}\|a_h\psi\| \\ &\leq \frac{1}{n_{\alpha,k}}\Big[\sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p-h,k}\Big]^{1/2}\Big[\sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}} \delta_{p-h,k}\|a_h\psi\|^2\Big]^{1/2} \leq \langle\psi,\mathcal{N}(B_{\mathrm{F}}\cap B_\alpha)\psi\rangle^{1/2},\end{aligned}$$

where we used that $\sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}\cap \mathrm{B}_\alpha}}} \delta_{p-h,k} = n_{\alpha,k}^2$. This proves (5.5).
We will use (5.5) together with Cauchy–Schwarz to prove the first inequality of (5.6),

$$\begin{aligned}\Big\|\sum_{\alpha\in\mathcal{I}_k} \overline{f(\alpha)}c_\alpha(k)\psi\Big\|^2 &\leq \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2 \sum_{\alpha'\in\mathcal{I}_k}\|c_{\alpha'}(k)\psi\|^2 \\ &\leq \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2 \sum_{\alpha'\in\mathcal{I}_k}\|\mathcal{N}(B_{\mathrm{F}}\cap B_{\alpha'})^{1/2}\psi\|^2 \leq \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\langle\psi,\mathcal{N}\psi\rangle.\end{aligned}$$

It remains to prove the second inequality of (5.6). Using Lemma 5.1, we find

$$\begin{aligned}&\Big\|\sum_{\alpha\in\mathcal{I}_k} f(\alpha)c_\alpha^*(k)\psi\Big\|^2 \\ &= \sum_{\alpha,\beta\in\mathcal{I}_k}\overline{f(\alpha)}f(\beta)\langle\psi,c_\beta^*(k)c_\alpha(k)\psi\rangle + \sum_{\alpha,\beta\in\mathcal{I}_k}\overline{f(\alpha)}f(\beta)\langle\psi,[c_\alpha(k),c_\beta^*(k)]\psi\rangle \\ &= \Big\|\sum_{\alpha\in\mathcal{I}_k}\overline{f(\alpha)}c_\alpha(k)\psi\Big\|^2 + \sum_{\alpha,\beta\in\mathcal{I}_k}\overline{f(\alpha)}f(\beta)\langle\psi,\delta_{\alpha,\beta}(1+\mathcal{E}_\alpha(k,k))\psi\rangle \\ &\leq \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\sum_{\alpha'\in\mathcal{I}_k}\|c_{\alpha'}(k)\psi\|^2 + \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\|\psi\|^2 + \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\langle\psi,\mathcal{E}_\alpha(k,k)\psi\rangle. \qquad (5.7)\end{aligned}$$

Recall from (5.4) that for $\alpha\in\mathcal{I}_k^+$ we have

$$\mathcal{E}_\alpha(k,k) = -\frac{1}{n_{\alpha,k}^2}\sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}}\delta_{p-h,k}a_h^*a_h - \frac{1}{n_{\alpha,k}^2}\sum_{\substack{p\in B_{\mathrm{F}}^c\cap B_\alpha \\ h\in B_{\mathrm{F}}\cap B_\alpha}}\delta_{p-h,k}a_p^*a_p.$$

We immediately see that $\langle\psi,\mathcal{E}_\alpha(k,k)\psi\rangle\leq 0$ (because the operators $a_k^*a_k$ acts either as the identity or as the zero map). For $\alpha\in\mathcal{I}_k^-$ we replace k by $-k$ on the r.h.s. which produces again a negative semidefinite operator. Hence, we can drop the last summand in (5.7) for an upper bound. Together with the first bound of (5.6) we get

$$\Big\|\sum_{\alpha\in\mathcal{I}_k} f(\alpha)c_\alpha^*(k)\psi\Big\|^2 \leq \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\langle\psi,\mathcal{N}\psi\rangle + \sum_{\alpha\in\mathcal{I}_k}|f(\alpha)|^2\langle\psi,\psi\rangle.$$

□

5.2 The Trial State

We write the correlation Hamiltonian $\mathcal{H}_{\mathrm{corr}}$ in terms of the almost-bosonic pair operators $c^*_\alpha(k)$ and $c_\alpha(k)$. The trial state will be chosen to minimize the energy of the Hamiltonian treating the operators $c^*_\alpha(k)$ and $c_\alpha(k)$ as bosonic.

We want to approximate the correlation Hamiltonian as a quadratic Hamiltonian in terms of $c^*_\alpha(k)$ and $c_\alpha(k)$. We start by inserting the Decomposition (4.14) into (4.11) and find

$$Q^{\mathrm{B}}_N = \frac{1}{2N}\sum_{k\in\mathbb{Z}^3\setminus\{0\}}\hat{V}(k)\Big[2\sum_{\alpha\in\mathcal{I}^+_k}\sum_{\beta\in\mathcal{I}^+_k} n_{\alpha,k}n_{\beta,k}b^*_{\alpha,k}b_{\beta,k} + \sum_{\alpha\in\mathcal{I}^+_k}\sum_{\beta\in\mathcal{I}^+_{-k}} n_{\alpha,k}n_{\beta,-k}b^*_{\alpha,k}b^*_{\beta,-k} + \sum_{\alpha\in\mathcal{I}^+_{-k}}\sum_{\beta\in\mathcal{I}^+_k} n_{\alpha,-k}n_{\beta,k}b_{\alpha,-k}b_{\beta,k}\Big] + \text{error terms}.$$

The error terms contain at least one $\mathfrak{r}_k$-operator. Using Definition (4.15) of $v_\alpha(k)$, Definition (5.1) of the operators c and c^* and allowing to sum over Γ^{nor}, we have

$$\begin{aligned} Q^{\mathrm{B}}_N = \hbar\kappa^2\sum_{k\in\Gamma^{\mathrm{nor}}}|k|\hat{V}(k)\Big[&\sum_{\alpha\in\mathcal{I}^+_k}\sum_{\beta\in\mathcal{I}^+_k} v_\alpha(k)v_\beta(k)c^*_\alpha(k)c_\beta(k) \\ &+ \sum_{\alpha\in\mathcal{I}^-_k}\sum_{\beta\in\mathcal{I}^-_k} v_\alpha(-k)v_\beta(-k)c^*_\alpha(k)c_\beta(k) \\ &+ \sum_{\alpha\in\mathcal{I}^+_k}\sum_{\beta\in\mathcal{I}^-_k}\Big(v_\alpha(k)v_\beta(-k)c^*_\alpha(k)c^*_\beta(k) + \text{h.c.}\Big)\Big] + \text{error terms} \end{aligned} \tag{5.8}$$

where $\kappa = (3/4\pi)^{1/3} + \mathcal{O}(N^{-1/3})$. It remains to rewrite the operator $\mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v)$ in terms of c^*_α and c_α. We neglect the contribution of the constant direct terms and of the exchange operator X on the r.h.s. of (4.3) (they will be proven to be small). For $\alpha \in \mathcal{I}^+_k$ we approximate

$$\begin{aligned} \mathrm{d}\Omega(uhu - \overline{v}\overline{h}v)c^*_\alpha(k)\Omega &\simeq \frac{1}{n_{\alpha,k}}\sum_{\substack{p\in B^c_{\mathrm{F}}\cap B_\alpha\\ h\in B_{\mathrm{F}}\cap B_\alpha}}\frac{\hbar^2(|p|^2-|h|^2)}{2}a^*_pa^*_h\delta_{p-h,k}\Omega \\ &= \frac{1}{n_{\alpha,k}}\sum_{\substack{p\in B^c_{\mathrm{F}}\cap B_\alpha\\ h\in B_{\mathrm{F}}\cap B_\alpha}}\frac{\hbar^2(p-h)\cdot(p+h)}{2}a^*_pa^*_h\delta_{p-h,k}\Omega \\ &\simeq \frac{1}{n_{\alpha,k}}\sum_{\substack{p\in B^c_{\mathrm{F}}\cap B_\alpha\\ h\in B_{\mathrm{F}}\cap B_\alpha}}\frac{\hbar^2k\cdot 2\omega_\alpha}{2}a^*_pa^*_h\delta_{p-h,k}\Omega = \hbar^2k\cdot\omega_\alpha c^*_\alpha(k)\Omega, \end{aligned}$$

where we used that for $p, h \in B_\alpha$, $p \simeq \omega_\alpha \simeq h$. A similar computation for $\alpha \in \mathcal{I}^-_k$ shows that

$$\mathrm{d}\Omega(uhu - \overline{v}\overline{h}v)c^*_\alpha(k)\Omega \simeq \hbar^2|k\cdot\omega_\alpha|c^*_\alpha(k)\Omega \tag{5.9}$$

for all $\alpha \in \mathcal{I}_k$. If the operators $c^*_\alpha(k), c_\alpha(k)$ were bosonic creation and annihilation operators, satisfying canonical commutation relations, and if $\mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v)$ were quadratic in these operators, (5.9) leads to

$$\mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v) \simeq \hbar^2 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha\in\mathcal{I}_k} |k\cdot\omega_\alpha| c^*_\alpha(k) c_\alpha(k).$$

We restrict our attention to states with few particle number to ensure that $c^*_\alpha(k)$ and $c_\alpha(k)$ behave almost bosonic. The Equations (5.8) and (5.9) show that the correlation Hamiltonian is approximated by a Hamiltonian of the form

$$\mathcal{H} = \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k| h_{\mathrm{eff}}(k) \tag{5.10}$$

with

$$\begin{aligned} h_{\mathrm{eff}} = \sum_{\alpha\in\mathcal{I}_k} u^2_\alpha(k) c^*_\alpha(k) c_\alpha(k) + g(k)\Big[\Big(\sum_{\alpha\in\mathcal{I}^+_k}\sum_{\beta\in\mathcal{I}^-_k} v_\alpha(k) v_\beta(-k) c^*_\alpha(k) c^*_\beta(k) + \mathrm{h.c.}\Big) \\ + \sum_{\alpha\in\mathcal{I}^+_k}\sum_{\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) c^*_\alpha(k) c_\beta(k) + \sum_{\alpha\in\mathcal{I}^-_k}\sum_{\beta\in\mathcal{I}^-_k} v_\alpha(-k) v_\beta(-k) c^*_\alpha(k) c^*_\beta(k)\Big] \end{aligned} \tag{5.11}$$

where we defined

$$u_\alpha(k) := |\hat{k}\cdot\hat{\omega}_\alpha|^{1/2}, \quad g(k) := \kappa\hat{V}(k). \tag{5.12}$$

The problem is that the particle–hole pair operators $c^*_\alpha(k)$ and $c_\alpha(k)$ are not exactly bosonic. If they were, the effective Hamiltonian $\mathcal{H}_{\mathrm{eff}}$ could be diagonalized via a bosonic Bogoliubov transformation and the ground state of (5.10) would be given by

$$\xi = \exp\Big[\frac{1}{2}\sum_{k\in\Gamma^{\mathrm{nor}}}\sum_{\alpha,\beta\in\mathcal{I}_k} K_{\alpha,\beta}(k) c^*_\alpha(k) c^*_\beta(k) - \mathrm{h.c.}\Big]\Omega, \tag{5.13}$$

where, for every $k \in \Gamma^{\mathrm{nor}}$, $K(k)$ is the $2I_k \times 2I_k$ matrix (with $I_k := |\mathcal{I}^+_k| = |\mathcal{I}^-_k|$) defined by

$$K(k) := \log|S^T_1(k)|, \tag{5.14}$$

with

$$S_1(k) := \Big(D(k) + W(k) - \tilde{W}(k)\Big)^{-1/2} E(k)^{-1/2}, \tag{5.15}$$

and

$$E(k) := \Big((D(k) + W(k) - \tilde{W}(k))^{1/2}(D(k) + W(k) + \tilde{W}(k))(D(k) + W(k) - \tilde{W}(k))^{1/2}\Big)^{1/2}$$

and, recalling the Definition (4.15) of $v_\alpha(k)$,

$$\begin{aligned} D(k) &:= \mathrm{diag}(u^2_\alpha(k) : \alpha \in \mathcal{I}_k), \\ W_{\alpha,\beta}(k) &:= \begin{cases} g(k) v_\alpha(k) v_\beta(k) & \text{for } \alpha,\beta \in \mathcal{I}^+_k \\ g(k) v_\alpha(-k) v_\beta(-k) & \text{for } \alpha,\beta \in \mathcal{I}^-_k \\ 0 & \text{for } \alpha \in \mathcal{I}^+_k, \beta \in \mathcal{I}^-_k \text{ or } \alpha \in \mathcal{I}^-_k, \beta \in \mathcal{I}^+_k, \end{cases} \\ \tilde{W}_{\alpha,\beta}(k) &:= \begin{cases} g(k) v_\alpha(k) v_\beta(-k) & \text{for } \alpha \in \mathcal{I}^+_k, \beta \in \mathcal{I}^-_k \\ g(k) v_\alpha(-k) v_\beta(k) & \text{for } \alpha \in \mathcal{I}^-_k, \beta \in \mathcal{I}^+_k \\ 0 & \text{for } \alpha,\beta \in \mathcal{I}^+_k \text{ or } \alpha,\beta \in \mathcal{I}^-_k. \end{cases} \end{aligned} \tag{5.16}$$

The computation of this ground state can be found in [2]. However, the operators $c_\alpha^*(k)$ and $c_\alpha(k)$ are not exactly bosonic. Hence, the ground state of (5.9) is not given by (5.13) but by Lemma 5.1 we can suggest that the true ground state of $\mathcal{H}_{\text{corr}}$ will be energetically close to ξ provided that the number of fermions in ξ is small.

Motivated by this heuristic discussion, the trial state for the energy of the correlation Hamiltonian $\mathcal{H}_{\text{corr}}$ is defined as

$$\psi_{\text{trial}} := R_{\omega_{\text{pw}}} T\Omega, \qquad T := e^B, \qquad B := \frac{1}{2}\sum_{k\in\Gamma^{\text{nor}}}\sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} c_\alpha^*(k) c_\beta^*(k) - \text{h.c.}. \tag{5.17}$$

Notice that $B^* = -B$ so T is unitary and $\|\psi_{\text{trial}}\| = 1$. Our original system consists of N particles. Thus, only trial states with N particle are valid. We need to check that ψ_{trial} satisfies this property. Writing $\xi := R_{\omega_{\text{pw}}}^* \psi_{\text{trial}}$, we have

$$\mathcal{N}\psi_{\text{trial}} = R_{\omega_{\text{pw}}}\big[\sum_{p\in B_{\text{F}}^c} a_p^* a_p + \sum_{h\in B_{\text{F}}} a_h a_h^*\big]\xi = R_{\omega_{\text{pw}}}(\mathcal{N}_p - \mathcal{N}_h)\xi + N\psi_{\text{trial}},$$

where we used the identity $R_{\omega_{\text{pw}}}^* \sum_{h\in B_{\text{F}}} a_h^* a_h R_{\omega_{\text{pw}}} = \sum_{h\in B_{\text{F}}} a_h a_h^* = N - \sum_{h\in B_{\text{F}}} a_h^* a_h$ for the last equality. This shows that ψ_{trial} is an eigenvector of $\mathcal{N}$ with eigenvalue N if and only if ξ is an eigenvector of $\mathcal{N}_p - \mathcal{N}_h$ with eigenvalue 0. This is shown in the next lemma.

Lemma 5.3 (Particle–Hole Symmetry)**.** *For ξ as in (5.13) we have $(\mathcal{N}_p - \mathcal{N}_h)\xi = 0$.*

Proof. Let $\xi_\lambda = T_\lambda\Omega$ with $T_\lambda = e^{\lambda B}$ for $\lambda \in [0,1]$. Then $\xi_1 = \xi$ and $\xi_0 = \Omega$, and thus

$$\|(\mathcal{N}_p - \mathcal{N}_h)\xi\|^2 = \int_0^1 \mathrm{d}\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda}\langle \xi_\lambda, (\mathcal{N}_p - \mathcal{N}_h)^2 \xi_\lambda\rangle = \int_0^1 \mathrm{d}\lambda \langle \xi_\lambda, [(\mathcal{N}_p - \mathcal{N}_h)^2, B]\xi_\lambda\rangle = 0.$$

because $[\mathcal{N}_p - \mathcal{N}_h, c_\alpha^*(k)] = 0 = [\mathcal{N}_p - \mathcal{N}_h, c_\alpha(k)]$ (for each particle the operators c_α and c_α^* annihilate or create, there is a hole annihilated or created at the same time) implies $[\mathcal{N}_p - \mathcal{N}_h, B] = 0$. □

5.3 Approximate Bosonic Bogoliubov Transformations

The task of this section is to show some important properties of the operator T or more accurate, properties of the one-parameter family of unitary transformations $T_\lambda = e^{\lambda B}$, with B defined as in (5.17).

We want to show that we can reach the state ξ by the action of an approximate bosonic Bogoliubov transformation on the vacuum state Ω. This is the content of the following proposition. It shows that the action T_λ approximates a bosonic Bogoliubov transformation.

Proposition 5.4 (Approximate Bogoliubov Transformation)**.** *Let $\lambda \in [0,1]$. Let $l \in \Gamma^{\text{nor}}$ and $\gamma \in \mathcal{I}_l$. Then*

$$T_\lambda^* c_\gamma(l) T_\lambda = \sum_{\alpha\in\mathcal{I}_l} \cosh(\lambda K(l))_{\alpha,\gamma} c_\alpha(l) + \sum_{\alpha\in\mathcal{I}_l} \sinh(\lambda K(l))_{\alpha,\gamma} c_\alpha^*(l) + \mathfrak{E}_\gamma(\lambda, l),$$

where the error operator $\mathfrak{E}_\gamma(\lambda,l)$ satisfies, for all $\psi\in\mathcal{F}$, the bound

$$\Big[\sum_{\gamma\in\mathcal{I}_l}\|\mathfrak{E}_\gamma(\lambda,l)\psi\|^2\Big]^{1/2}\leq\frac{C}{\mathfrak{n}^2}N^\mu\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+2)^{3/2}T_\tau\psi\|e^{\lambda\|K(l)\|_{\mathrm{HS}}}\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}. \quad (5.18)$$

Here $\mathfrak{n}=N^{1/3-\delta/2}M^{-1/2}$, as defined in (4.16)*, and $\|K(k)\|_{\mathrm{HS}}$ denotes the Hilbert–Schmidt norm of the matrix $K(k)$. The same estimate holds for $\mathfrak{E}^*_\gamma(\lambda,l)$.*

Proof. We start from the Duhamel formula

$$T^*_\lambda c_\gamma(l)T_\lambda=c_\gamma(l)+\int_0^\lambda \mathrm{d}\tau T^*_\tau[c_\gamma(l),B]T_\tau.$$

Lemma 5.1 shows that the commutator is given by

$$[c_\gamma(l),B]=\sum_{k\in\Gamma^{\mathrm{nor}}}\frac{1}{2}\sum_{\alpha,\beta\in\mathcal{I}_k}K(k)_{\alpha,\beta}[c_\gamma(l),c^*_\alpha(k)c^*_\beta(k)]=\sum_{\alpha\in\mathcal{I}_l}K(l)_{\gamma,\alpha}c^*_\alpha(l)+\mathfrak{e}_\gamma(l)$$

where the error term is given by

$$\mathfrak{e}_\gamma(l):=\sum_{k\in\Gamma^{\mathrm{nor}}}\frac{\chi_{\mathcal{I}_k}(\gamma)}{2}\sum_{\alpha\in\mathcal{I}_k}K(k)_{\gamma,\alpha}(\mathcal{E}_\gamma(k,l)c^*_\alpha(k)+c^*_\alpha(k)\mathcal{E}_\gamma(k,l)), \quad (5.19)$$

with $\chi_{\mathcal{I}_k}$ the indicator function of the set $\mathcal{I}_k$ and $\mathcal{E}_\gamma(k,l)$ bounded as in (5.3). Thus,

$$T^*_\lambda c_\gamma(l)T_\lambda=c_\gamma(l)+\sum_{\alpha\in\mathcal{I}_k}K(l)_{\gamma,\alpha}\int_0^\lambda\mathrm{d}\tau T^*_\tau c^*_\alpha(l)T_\tau+\int_0^\lambda\mathrm{d}\tau T^*_\tau\mathfrak{e}_\gamma(l)T_\tau,$$

$$T^*_\lambda c^*_\gamma(l)T_\lambda=c^*_\gamma(l)+\sum_{\alpha\in\mathcal{I}_k}K(l)_{\gamma,\alpha}\int_0^\lambda\mathrm{d}\tau T^*_\tau c_\alpha(l)T_\tau+\int_0^\lambda\mathrm{d}\tau T^*_\tau\mathfrak{e}^*_\gamma(l)T_\tau.$$

We iterate n_0 times by plugging the second equation into the second summand on the r.h.s. of the first equation an so forth. The simplex integrals produce factors $1/n!$. Hence, we find

$$\begin{aligned}
T^*_\lambda c_\gamma T_\lambda = {}& c_\gamma(l)\\
&+\sum_{\alpha\in\mathcal{I}_l}\lambda K(l)_{\gamma,\alpha}c^*_\alpha(l)+\int_0^\lambda\mathrm{d}\tau_1T^*_{\tau_1}\mathfrak{e}_\gamma(l)T_{\tau_1}\\
&+\frac{1}{2!}\sum_{\alpha\in\mathcal{I}_l}\big(\lambda^2K(l)^2\big)_{\gamma,\alpha}c_\alpha(l)+\sum_{\alpha\in\mathcal{I}_l}K(l)_{\gamma,\alpha}\int_0^\lambda\mathrm{d}\tau_1\int_0^{\tau_1}\mathrm{d}\tau_2T^*_{\tau_2}\mathfrak{e}^*_\alpha(l)T_{\tau_2}\\
&+\frac{1}{3!}\sum_{\alpha\in\mathcal{I}_l}\big(\lambda^3K(l)^3\big)_{\gamma,\alpha}c^*_\alpha(l)+\sum_{\alpha\in\mathcal{I}_l}\big(K(l)^2\big)_{\gamma,\alpha}\int_0^\lambda\mathrm{d}\tau_1\int_0^{\tau_1}\mathrm{d}\tau_2\int_0^{\tau_2}\mathrm{d}\tau_3T^*_{\tau_3}\mathfrak{e}_\alpha(l)T_{\tau_3}\\
&+\dots\\
&+\sum_{\alpha\in\mathcal{I}_l}(K(l)^{n_0})_{\gamma,\alpha}\int_0^\lambda\mathrm{d}\tau_1\int_0^{\tau_1}\mathrm{d}\tau_2\dots\int_0^{\tau_{n_0-1}}\mathrm{d}\tau_{n_0}T^*_{\tau_{n_0}}c^\natural_\alpha(l)T_{\tau_{n_0}}
\end{aligned}$$

where $c^\natural_\alpha(l)$ means $c^*_\alpha(l)$ for n_0 odd, and $c_\alpha(l)$ for n_0 even. The left term on every line is the leading term, the right term on every line is an error term which will be estimated later. The very last term is the 'head' of the iteration after n_0 steps. We will show that the head vanishes as $n_0 \to \infty$. Taking all the c^* and c separately together, we reconstruct $\cosh(\lambda K(l))$ and $\sinh(\lambda K(l))$. We have

$$T^*_\lambda c_\gamma(l) T_\lambda = \sum_{\alpha\in\mathcal{I}_l} \cosh(\lambda K(l))_{\gamma,\alpha} c_\alpha(l) + \sum_{\alpha\in\mathcal{I}_l} \sinh(\lambda K(l))_{\gamma,\alpha} c^*_\alpha(l) + \mathfrak{E}_\gamma(\lambda, l)$$

where, for an arbitrary $n_0 \in \mathbb{N}$,

$$\begin{aligned}\mathfrak{E}_\gamma(\lambda,l) := &\sum_{\alpha\in\mathcal{I}_l}\sum_{n=0}^{n_0-1} (K(l)^n)_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau_1 \dots \int_0^{\tau_n} \mathrm{d}\tau_{n+1} T^*_{\tau_{n+1}} \mathfrak{e}^\natural_\alpha(l) T_{\tau_{n+1}} \\ &+ \sum_{\alpha\in\mathcal{I}_l} (K(l)^{n_0})_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \dots \int_0^{\tau_{n_0-1}} \mathrm{d}\tau_{n_0} T^*_{\tau_{n_0}} c^\natural_\alpha(l) T_{\tau_{n_0}} \\ &- \sum_{\alpha\in\mathcal{I}_l}\sum_{n=n_0}^{\infty} \frac{\lambda^n (K(l)^n)_{\gamma,\alpha}}{n!} c^\natural_\alpha(l).\end{aligned}$$

Notice that for any function $f : \mathbb{R} \to \mathbb{R}$ the simplex integration simplifies to

$$\int_0^\lambda \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \dots \int_0^{\tau_n} \mathrm{d}\tau_{n+1} f(\tau_{n+1}) = \int_0^\lambda \frac{(\lambda-\tau)^n}{n!} f(\tau)\mathrm{d}\tau.$$

Therefore, for all $\psi \in \mathcal{F}$ we have

$$\begin{aligned}&\|\mathfrak{E}_\gamma(\lambda,l)\psi\| \\ &\le \Big\| \sum_{\alpha\in\mathcal{I}_l}\sum_{n=0}^{n_0-1} (K(l)^n)_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^n}{n!} T^*_\tau \mathfrak{e}^\natural_\alpha(l) T_\tau \psi \Big\| \\ &\quad + \Big\| \sum_{\alpha\in\mathcal{I}_l} (K(l)^{n_0})_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^{n_0-1}}{(n_0-1)!} T^*_\tau c^\natural_\alpha(l) T_\tau \Big\| + \Big\| \sum_{\alpha\in\mathcal{I}_l}\sum_{n=n_0}^{\infty} \frac{\lambda^n (K(l)^n)_{\gamma,\alpha}}{n!} c^\natural_\alpha(l)\psi \Big\|.\end{aligned}$$

Using the explicit Expression (5.19) for $\mathfrak{e}_\alpha^\natural(l)$ we can controll $\|\mathfrak{E}_\gamma(\lambda,l)\psi\|$ by

$$\begin{aligned}
&\Big\| \sum_{\alpha\in\mathcal{I}_l} \sum_{n=0}^{n_0-1} (K(l)^n)_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^n}{n!} \sum_{k\in\Gamma^{\mathrm{nor}}} \frac{\chi_{\mathcal{I}_k}(\alpha)}{2} \sum_{\delta\in\mathcal{I}_k} K(k)_{\alpha,\delta} T_\tau^* (\mathcal{E}_\alpha(k,l) c_\delta^*(k))^\natural T_\tau \psi \Big\| \\
&+ \Big\| \sum_{\alpha\in\mathcal{I}_l} \sum_{n=0}^{n_0-1} (K(l)^n)_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^n}{n!} \sum_{k\in\Gamma^{\mathrm{nor}}} \frac{\chi_{\mathcal{I}_k}(\alpha)}{2} \sum_{\delta\in\mathcal{I}_k} K(k)_{\alpha,\delta} T_\tau^* (c_\delta^*(k) \mathcal{E}_\alpha(k,l))^\natural T_\tau \psi \Big\| \\
&+ \Big\| \sum_{\alpha\in\mathcal{I}_l} (K(l)^{n_0})_{\gamma,\alpha} \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^{n_0-1}}{(n_0-1)!} T_\tau^* c_\alpha^\natural(l) T_\tau \Big\| \\
&+ \Big\| \sum_{\alpha\in\mathcal{I}_l} \sum_{n=n_0}^{\infty} \frac{\lambda^n (K(l)^n)_{\gamma,\alpha}}{n!} c_\alpha^\natural(l) \psi \Big\| \\
&=: \mathrm{A}_\gamma + \mathrm{B}_\gamma + \mathrm{C}_\gamma + \mathrm{D}_\gamma.
\end{aligned}$$

We start by estimating B_γ. We will neglect the symbol $\natural$ because the bounds are the same whether for the operator or its adjoint. Since T_λ is unitary we can drop T_λ^*. Using (5.6), we get

$$\begin{aligned}
\mathrm{B}_\gamma &\leq \sum_{\alpha\in\mathcal{I}_l} \sum_{n=0}^{\infty} |(K(l)^n)_{\gamma,\alpha}| \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^n}{n!} \sum_{k\in\Gamma^{\mathrm{nor}}} \frac{\chi_{\mathcal{I}_k}(\alpha)}{2} \Big\| \sum_{\delta\in\mathcal{I}_k} K(k)_{\alpha,\delta} c_\delta^*(k) \mathcal{E}_\alpha(k,l) T_\tau \psi \Big\| \\
&\leq \sum_{\alpha\in\mathcal{I}_l} \sum_{n=0}^{\infty} |(K(l)^n)_{\gamma,\alpha}| \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^n}{n!} \sum_{k\in\Gamma^{\mathrm{nor}}} \frac{\chi_{\mathcal{I}_k}(\alpha)}{2} \Big[\sum_{\delta\in\mathcal{I}_k} |K(k)_{\alpha,\delta}|^2 \Big]^{1/2} \\
&\quad \times \|(\mathcal{N}+1)^{1/2} \mathcal{E}_\alpha(k,l) T_\tau \psi\|.
\end{aligned}$$

Since $\mathcal{E}_\alpha(k,l)$ and $\mathcal{N}$ commute, we can pull $\mathcal{E}_a(k,l)$ through $(\mathcal{N}+1)^{1/2}$ to the front. Then, by using (5.3), we find

$$\begin{aligned}
\mathrm{B}_\gamma &\leq \sum_{\alpha\in\mathcal{I}_l} \sum_{n=0}^{\infty} |(K(l)^n)_{\gamma,\alpha}| \int_0^\lambda \mathrm{d}\tau \frac{(\lambda-\tau)^n}{n!} \sum_{k\in\Gamma^{\mathrm{nor}}} \chi_{\mathcal{I}_k}(\alpha) \Big[\sum_{\delta\in\mathcal{I}_k} |K(k)_{\alpha,\delta}|^2 \Big]^{1/2} \\
&\quad \times \frac{\|\mathcal{N}(\mathcal{N}+1)^{1/2} T_\tau \psi\|}{n_{\alpha,k} n_{\alpha,l}} \\
&\leq \frac{\sup_{\tau\in[0,\lambda]} \|(\mathcal{N}+1)^{3/2} T_\tau \psi\|}{\mathfrak{n}^2} \\
&\quad \times \sum_{n=0}^{\infty} \frac{\lambda^{n+1}}{(n+1)!} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha\in\mathcal{I}_l\cap\mathcal{I}_k} |(K(l)^n)_{\gamma,\alpha}| \Big[\sum_{\delta\in\mathcal{I}_k} |K(k)_{\alpha,\delta}|^2 \Big]^{1/2} \\
&\leq \frac{\sup_{\tau\in[0,\lambda]} \|(\mathcal{N}+1)^{3/2} T_\tau \psi\|}{\mathfrak{n}^2} \Big[\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} \chi_{\mathcal{I}_k}(\gamma) \Big[\sum_{\delta\in\mathcal{I}_k} |K(k)_{\gamma,\delta}|^2 \Big]^{1/2} + \sum_{n=1}^{\infty} \frac{\lambda^{n+1}}{(n+1)!} \\
&\quad \times \Big[\sum_{\alpha\in\mathcal{I}_l\cap\mathcal{I}_k} |(K(l)^n)_{\gamma,\alpha}|^2 \Big]^{1/2} \sum_{k\in\Gamma^{\mathrm{nor}}} \|K(k)\|_{\mathrm{HS}} \Big]
\end{aligned}$$

where we used that $n_{\alpha,k} \geq C\mathfrak{n}$, we separated the term with $n = 0$ and, for $n \geq 1$, we applied Cauchy–Schwarz to the sum over α.
Using Cauchy–Schwarz, we can do the following estimates

$$\begin{aligned}\sum_{\gamma\in\mathcal{I}_l}\Big[\sum_{k\in\Gamma^{\mathrm{nor}}}\chi_{\mathcal{I}_k}(\gamma)\Big[\sum_{\delta\in\mathcal{I}_k}|K(k)_{\gamma,\delta}|^2\Big]^{1/2}\Big]^2 &\leq \sum_{\gamma\in\mathcal{I}_l\cap\mathcal{I}_k}\Big[\sum_{k\in\Gamma^{\mathrm{nor}}}\sum_{\delta\in\mathcal{I}_k}|K(k)_{\gamma,\delta}|^2\Big]\Big[\sum_{k\in\Gamma^{\mathrm{nor}}}1\Big]\\ &\leq CN^{\mu}\sum_{k\in\Gamma^{\mathrm{nor}}}\sum_{\gamma,\delta\in\mathcal{I}_k}|K(k)_{\gamma,\delta}|^2\\ &\leq CN^{\mu}\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}^2 \qquad (5.20)\end{aligned}$$

and

$$\begin{aligned}&\sum_{\gamma\in\mathcal{I}_l}\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\Big[\sum_{\alpha\in\mathcal{I}_l\cap\mathcal{I}_k}|(K(l)^n)_{\gamma,\alpha}|^2\Big]^{1/2}\Big]^2\\ \leq&\sum_{\gamma\in\mathcal{I}_l}\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)}\frac{1}{\|K(l)\|_{\mathrm{HS}}^n}\sum_{\alpha\in\mathcal{I}_l\cap\mathcal{I}_k}|(K(l))^n_{\alpha,\gamma}|^2\Big]\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\|K(l)\|_{\mathrm{HS}}^n\Big]\\ \leq&\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\frac{1}{\|K(l)\|_{\mathrm{HS}}^n}\|K(l)^n\|_{\mathrm{HS}}^2\Big]\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\|K(l)\|_{\mathrm{HS}}^n\Big]\\ \leq&\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\|K(l)\|_{\mathrm{HS}}^n\Big]^2. \qquad (5.21)\end{aligned}$$

Using (5.20) and (5.21), we find

$$\begin{aligned}\Big[\sum_{\gamma\in\mathcal{I}_l}\mathrm{B}_{\gamma}^2\Big]^{1/2} &\leq CN^{\mu/2}\frac{\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+1)^{3/2}T_{\tau}\psi\|}{\mathfrak{n}^2}\\ &\quad\times\Big[\lambda\Big[\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}^2\Big]^{1/2}+\Big[\sum_{n=1}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\|K(l)\|_{\mathrm{HS}}^n\Big]\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}\Big]\\ &\leq CN^{\mu/2}\frac{\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+1)^{3/2}T_{\tau}\psi\|}{\mathfrak{n}^2}\Big[\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}\Big]\Big[\frac{e^{\lambda\|K(l)\|_{\mathrm{HS}}}-1}{\|K(l)\|_{\mathrm{HS}}}\Big]\\ &\leq CN^{\mu/2}\frac{\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+1)^{3/2}T_{\tau}\psi\|}{\mathfrak{n}^2}e^{\lambda\|K(l)\|_{\mathrm{HS}}}\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}.\end{aligned}$$

The last bound can be proven by considering separately the following cases:

- $\|K(l)\|_{\mathrm{HS}} \geq 1$, then the bound is obvious, and
- $\|K(l)\|_{\mathrm{HS}} < 1$, then we consider the function $f(\lambda) := \frac{e^{\lambda\|K(l)\|_{\mathrm{HS}}}-1}{\|K(l)\|_{\mathrm{HS}}} - e^{\lambda\|K(l)\|_{\mathrm{HS}}}$. This function is monotonically increasing because $f'(\lambda) > 0$ and since $\lambda \in [0,1]$ it suffices to check that $f(1) \leq 0$ which is clearly true.

The term A_γ can be estimated similar, using first (5.3) and afterwards (5.6):

$$\begin{aligned}\mathrm{A}_\gamma &\leq \sum_{\alpha\in\mathcal{I}_l}\sum_{n=0}^{\infty}|(K(l)^n)_{\gamma,\alpha}|\int_0^\lambda \mathrm{d}\tau\frac{(\lambda-\tau)^n}{n!}\sum_{k\in\Gamma^{\mathrm{nor}}}\frac{\chi_{\mathcal{I}_k}(\alpha)}{2}\Big\|\sum_{\delta\in\mathcal{I}_k}K(k)_{\alpha,\delta}\mathcal{E}_\alpha(k,l)c_\delta^*(k)T_\tau\psi\Big\|\\ &\leq \sum_{\alpha\in\mathcal{I}_l}\sum_{n=0}^{\infty}|(K(l)^n)_{\gamma,\alpha}|\int_0^\lambda \mathrm{d}\tau\frac{(\lambda-\tau)^n}{n!}\sum_{k\in\Gamma^{\mathrm{nor}}}\frac{\chi_{\mathcal{I}_k}(\alpha)}{\mathfrak{n}^2}\Big\|\sum_{\delta\in\mathcal{I}_k}K(k)_{\alpha,\delta}\mathcal{N}c_\delta^*(k)T_\tau\psi\Big\|.\end{aligned}$$

Pulling $c_\delta^*(k)$ through $\mathcal{N}$, using that $[\mathcal{N},c_\delta^*(k)]=2c_\delta^*(k)$, we get

$$\begin{aligned}\mathrm{A}_\gamma &\leq \sum_{\alpha\in\mathcal{I}_l}\sum_{n=0}^{\infty}|(K(l)^n)_{\gamma,\alpha}|\int_0^\lambda \mathrm{d}\tau\frac{(\lambda-\tau)^n}{n!}\sum_{k\in\Gamma^{\mathrm{nor}}}\frac{\chi_{\mathcal{I}_k}(\alpha)}{\mathfrak{n}^2}\Big\|\sum_{\delta\in\mathcal{I}_k}K(k)_{\alpha,\delta}c_\delta^*(k)(\mathcal{N}+2)T_\tau\psi\Big\|\\ &\leq \sum_{\alpha\in\mathcal{I}_l}\sum_{n=0}^{\infty}|(K(l)^n)_{\gamma,\alpha}|\int_0^\lambda \mathrm{d}\tau\frac{(\lambda-\tau)^n}{n!}\sum_{k\in\Gamma^{\mathrm{nor}}}\frac{\chi_{\mathcal{I}_k}(\alpha)}{\mathfrak{n}^2}\Big[\sum_{\delta\in\mathcal{I}_k}|K(k)_{\alpha,\delta}|^2\Big]^{1/2}\\ &\quad\times\|(\mathcal{N}+1)^{1/2}(\mathcal{N}+2)T_\tau\psi\|\leq C\frac{\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+2)^{3/2}T_\tau\psi\|}{\mathfrak{n}^2}\sum_{n=0}^{\infty}\frac{\lambda^{n+1}}{(n+1)!}\\ &\quad\times\sum_{k\in\Gamma^{\mathrm{nor}}}\sum_{\alpha\in\mathcal{I}_l\cap\mathcal{I}_k}|(K(l)^n)_{\gamma,\alpha}|\Big[\sum_{\delta\in\mathcal{I}_k}|K(k)_{\alpha,\delta}|^2\Big]^{1/2}.\end{aligned}$$

Using the same bounds as for B_γ yields

$$\Big[\sum_{\gamma\in\mathcal{I}_l}\mathrm{A}_\gamma^2\Big]^{1/2}\leq CN^{\mu/2}\frac{\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+2)^{3/2}T_\tau\psi\|}{\mathfrak{n}^2}e^{\lambda\|K(l)\|_{\mathrm{HS}}}\sum_{k\in\Gamma^{\mathrm{nor}}}\|K(k)\|_{\mathrm{HS}}.$$

Using (5.6), the term C_γ can be controlled by

$$\begin{aligned}\mathrm{C}_\gamma &\leq \Big\|\sum_{\alpha\in\mathcal{I}_l}(K(l)^{n_0})_{\gamma,\alpha}\int_0^\lambda \mathrm{d}\tau\frac{(\lambda-\tau)^{n_0-1}}{(n_0-1)!}T_\tau^*c_\alpha^\natural(l)T_\tau\Big\|\\ &\leq \int_0^\lambda \mathrm{d}\tau\frac{(\lambda-\tau)^{n_0-1}}{(n_0-1)!}\Big\|\sum_{\alpha\in\mathcal{I}_l}(K(l)^{n_0})_{\gamma,\alpha}c_\alpha^\natural(l)T_\tau\psi\Big\|\\ &\leq \frac{\lambda^{n_0}}{n_0!}\Big[\sum_{\alpha\in\mathcal{I}_l}|(K(l)^{n_0})_{\gamma,\alpha}|^2\Big]^{1/2}\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+1)^{1/2}T_\tau\psi\|.\end{aligned}$$

From this it follows that

$$\Big[\sum_{\gamma\in\mathcal{I}_l}\mathrm{C}_\gamma^2\Big]^{1/2}\leq C\frac{\lambda^{n_0}\|K(l)\|_{\mathrm{HS}}^{n_0}}{n_0!}\sup_{\tau\in[0,\lambda]}\|(\mathcal{N}+1)^{1/2}T_\tau\psi\|.$$

The last term D_γ can be bounded by

$$\mathrm{D}_\gamma\leq\sum_{n\geq n_0}\frac{\lambda^n}{n!}\Big\|\sum_{\alpha\in\mathcal{I}_l}(K(l)^n)_{\gamma,\alpha}c_\alpha^\natural(l)\psi\Big\|\leq\sum_{n\geq n_0}\frac{\lambda^n}{n!}\Big[\sum_{\alpha\in\mathcal{I}_l}|(K(l)^n)_{\gamma,\alpha}|^2\Big]^{1/2}\|(\mathcal{N}+1)^{1/2}\psi\|$$

which is used to get

$$\Big[\sum_{\gamma\in\mathcal{I}_l} \mathrm{D}_\gamma^2\Big]^{1/2} \leq C \sum_{n\geq n_0} \frac{\lambda^n \|K(l)\|_{\mathrm{HS}}^n}{n!} \|(\mathcal{N}+1)^{1/2}\psi\|.$$

All these bounds holds for any $n_0 \in \mathbb{N}$, so we get

$$\Big[\sum_{\gamma\in\mathcal{I}_l} \|\mathfrak{E}_\gamma(\lambda,l)\psi\|^2\Big]^{1/2} \leq CN^\mu \frac{\sup_{\tau\in[0,\lambda]} \|\mathcal{N}+2)^{3/2} T_\tau \psi\|}{\mathfrak{n}^2} e^{\lambda\|K(l)\|_{\mathrm{HS}}} \sum_{k\in\Gamma^{\mathrm{nor}}} \|K(k)\|_{\mathrm{HS}}.$$

□

To understand better the bound for the error of the approximate Bogoliubov transformation (5.18), we need appropriate bounds for the Hilbert–Schmidt norm of the matrix $K(k)$, defined in (5.14). We will see that it is important that $K(k) = 0$ for $|k| > N^\mu$. This is the content of the next lemma.

Lemma 5.5 (Bound on the Bogoliubov Kernel)**.** *Let $k \in \Gamma^{\mathrm{nor}}$. Then the matrices $E(k)$, $D(k)+W(k)-\tilde{W}(k)$ and $D(k)+W(k)+\tilde{W}(k)$, all defined in* (5.16)*, are strictly positive. Let $K(k)$ be defined by* (5.14)*. Then we have*

$$\|K(k)\|_{\mathrm{HS}} \leq \|K(k)\|_{\mathrm{tr}} \leq C\hat{V}(k), \tag{5.22}$$

where $\|K(k)\|_{\mathrm{tr}}$ denotes the trace norm of the matrix $K(k)$.

Proof. Recall that $I_k = |\mathcal{I}_k^+| = |\mathcal{I}_k^-|$ and that the matrix $K(k)$ is symmetric and has size $2I_k \times 2I_k$. In this proof, all quantities depend on the same k, so we drop this dependence for simplicity, writing e.g., I for I_k.
To exhibit the block structure of the matrices, we map the indices $\mathcal{I}_k^+$ to $\{1,\ldots,I\}$, and the indices $\mathcal{I}_k^-$ to $\{I+1,\ldots,2I\}$. There are many such mappings, but due to the reflection symmetry of the patches ($B_{\alpha+M/2} = -B_\alpha$ and $\omega_{\alpha+M/2} = -\omega_a$ in the original numbering), we can choose one such that $v_\alpha(k) = v_{\alpha+I}(-k)$. This implies that

$$W = \begin{pmatrix} b & 0 \\ 0 & b \end{pmatrix}, \quad \tilde{W} = \begin{pmatrix} 0 & b \\ b & 0 \end{pmatrix}, \tag{5.23}$$

where $b_{\alpha,\beta} = g v_a v_\beta$ defines an $I \times I$-matrix. In Dirac notation, where $|v\rangle\langle v|$ is the orthogonal projection onto $v = (v_1,\ldots,v_I)$, we have $b = g\,|v\rangle\langle v| \in \mathbb{C}^{I\times I}$. Also $D_{\alpha,\alpha} = |\hat{k}\cdot\hat{\omega}_a|$ is invariant under reflection at the origin and so D simplifies to

$$D = \begin{pmatrix} d & 0 \\ 0 & d \end{pmatrix}, \quad d = \mathrm{diag}(u_\alpha^2, \alpha = 1,\ldots,I).$$

Recalling the definition of the index set $\mathcal{I}_k^+$ we notice that $u_\alpha^2 \geq N^{-\delta}$ for all $\alpha \in \{1,\ldots,I\}$, and thus d is invertible. Since $b \geq 0$ (because $g \geq 0$), we find $d + 2b \geq d > 0$. Hence also $d+2b$ is invertible. To simplify the computation further, let

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & \mathbb{I} \\ \mathbb{I} & -\mathbb{I} \end{pmatrix},$$

where $\mathbb{I}$ is the $I \times I$-identity matrix. Obviously $U^T = U = U^{-1}$, and it simultaneously blockdiagonalizes

$$U^T(D+W+\tilde{W})U = \begin{pmatrix} d+2b & 0 \\ 0 & d \end{pmatrix}, \quad U^T(D+W-\tilde{W})U = \begin{pmatrix} d & 0 \\ 0 & d+2b \end{pmatrix} \tag{5.24}$$

This shows that $D+W+\tilde{W}$ and $D+W-\tilde{W}$ are strictly positive, thus invertible, and have a positive square root. We also find

$$U^T E U = \begin{pmatrix} [d^{1/2}(d+2b)d^{1/2}]^{1/2} & 0 \\ 0 & [(d+2b)^{1/2}d(d+2b)^{1/2}]^{1/2} \end{pmatrix}.$$

Both blocks are strictly positive. Therefore, E is invertible and has a strictly positive operator square root. Now consider

$$|S_1|^2 = S_1^T S_1 = E^{-1/2}(D+W-\tilde{W})E^{-1/2}.$$

We find

$$U^T|S_1|^2 U = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} \tag{5.25}$$

with

$$\begin{aligned} A_1 &:= \Big[d^{1/2}(d+2b)d^{1/2}\Big]^{-1/4} d \Big[d^{1/2}(d+2b)d^{1/2}\Big]^{-1/4}, \\ A_2 &:= \Big[(d+2b)^{1/2}d(d+2b)^{1/2}\Big]^{-1/4}(d+2b)\Big[(d+2b)^{1/2}d(d+2b)^{1/2}\Big]^{-1/4}. \end{aligned} \tag{5.26}$$

Since b is a positive operator, using operator monotonicity of the inverse and the square root, we find

$$d^{1/2}\Big[d^{1/2}(d+2b)d^{1/2}\Big]^{-1/2} d^{1/2} \leq \mathbb{I}.$$

Using the equality of the spectra $\sigma(AB) = \sigma(BA)$ for positive operators A and B, we conclude that

$$\sigma(A_1) = \sigma\bigg(d\Big[d^{1/2}(d+2b)d^{1/2}\Big]^{-1/2}\bigg) = \sigma\bigg(d^{1/2}\Big[d^{1/2}(d+2b)d^{1/2}\Big]d^{1/2}\bigg)$$

and therefore,

$$A_1 \leq \mathbb{I}. \tag{5.27}$$

Arguing similarly, we find that

$$\mathbb{I} \leq A_2. \tag{5.28}$$

We introduce the polar decomposition $S_1 = O|S_1|$. The matrix O is a partial isometry, but since S_1 is invertible, O is actually an orthogonal matrix. Then $|S_1^T|^2 = S_1 S_1^T = O|S_1||S_1|^T O^T = O|S_1|^2 O^T$ because $|S_1|^T = |S_1|$. This implies

$$\|K\|_{\mathrm{tr}} = \|\log|S_1^T|\|_{\mathrm{tr}} = \frac{1}{2}\|\log|S_1^T|^2\|_{\mathrm{tr}} = \frac{1}{2}\|\log O|S_1|^2 O^T\|_{\mathrm{tr}} = \frac{1}{2}\|\log|S_1\|^2\|_{\mathrm{tr}}.$$

Using furthermore the block diagonalization (5.25), we find

$$\|K\|_{\mathrm{tr}} = \frac{1}{2}\|U^T \log|S_1|^2 U\|_{\mathrm{tr}} = \frac{1}{2}\|\log\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}\|_{\mathrm{tr}} = \frac{1}{2}\|\log A_1\|_{\mathrm{tr}} + \frac{1}{2}\|\log A_2\|_{\mathrm{tr}}.$$

The Equations (5.27) and (5.28) imply that $\log A_1 \leq 0$ and $\log A_2 \geq 0$. Hence,

$$\|K\|_{\mathrm{tr}} = \frac{1}{2}(-\mathrm{tr}\log A_1 + \mathrm{tr}\log A_2) = \frac{1}{2}(-\log\det A_1 + \log\det A_2).$$

From Definition (5.26), we get

$$\begin{aligned}\|K\|_{\mathrm{tr}} &= \frac{1}{2}\Big(\log\det(d+2b) - \log\det d\Big) = \log\det\Big(\mathbb{I} + 2d^{-1/2}bd^{-1/2}\Big)\\ &\leq 2\mathrm{tr}\; d^{-1/2}bd^{-1/2} = 2g\langle v, d^{-1}v\rangle = 2g\sum_{\alpha=1}^{I}\frac{v_a^2}{u_\alpha^2} \leq Cg = C\kappa\hat{V}(k)\end{aligned}$$

where we used Proposition 4.1, which implies $v_\alpha^2 \leq CM^{-1}u_\alpha^2$. (Recall also $I \leq M/2$.) □

To control the error term (5.18) completely we still need to estimate the expectation of the operator $(\mathcal{N}+2)^{3/2}$ in the state $T_\tau\psi$. The bound follows from the proposition below.

Proposition 5.6 (Bound on the Number of Fermions)**.** *For all $n \in \mathbb{N}$ and for all $\psi \in \mathcal{F}$ we have (for a constant C not depending on n)*

$$\sup_{\lambda\in[0,1]}\langle T_\lambda\psi, (\mathcal{N}+1)^n T_\lambda\psi\rangle \leq e^{Cn}\langle\psi, (\mathcal{N}+5)^n\psi\rangle.$$

Proof. Form the CAR (2.8) we get

$$[\mathcal{N}, c_\alpha^*(k)] = 2c_\alpha^*(k) \quad \text{and} \quad c_\alpha^*(k)c_\beta^*(l)(\mathcal{N}+4) = \mathcal{N}c_\alpha^*(k)c_\beta^*(l).$$

This equality implies that for all $l \in \mathbb{N}$

$$c_\alpha^*(k)c_\beta^*(k)(\mathcal{N}+5)^l = (\mathcal{N}+1)^l c_\alpha^*(k)c_\beta^*(k). \tag{5.29}$$

We calculate the derivative w.r.t. λ of the expectation value of $(\mathcal{N}+5)^n$

$$\begin{aligned}&\left|\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle T_\lambda\psi, (\mathcal{N}+5)^n T_\lambda\psi\rangle\right| = \left|\langle T_\lambda\psi, (-B(\mathcal{N}+5)^n + (\mathcal{N}+5)^n B)T_\lambda\psi\rangle\right|\\ =&\left|\langle T_\lambda\psi, [B, (\mathcal{N}+5)^n]T_\lambda\psi\rangle\right| = \left|\langle T_\lambda\psi, \sum_{j=0}^{n-1}(\mathcal{N}+5)^j[\mathcal{N}, B](\mathcal{N}+5)^{n-j-1}T_\lambda\psi\rangle\right|\end{aligned}$$

where we have used that $B^* = -B$ and that for two operators A and B the following identity holds $A^nB = BA^n + \sum_{j=0}^{n-1}A^j[A,B]A^{n-1-j}$. Using Definition (5.17) for B and

the fact that $[\mathcal{N}, c_\beta(k)c_\alpha(k)]^* = -[\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)]$ yields

$$
\begin{aligned}
&= \Big| \langle T_\lambda\psi, \sum_{j=0}^{n-1} (\mathcal{N}+5)^j \frac{1}{2} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} [\mathcal{N}, c_\alpha^*(k)c_\beta^*(k) - \mathrm{h.c.}] (\mathcal{N}+5)^{n-j-1} T_\lambda\psi\rangle \Big| \\
&= \Big| \frac{1}{2} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} \sum_{j=0}^{n-1} \langle (\mathcal{N}+5)^j [\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)] (\mathcal{N}+5)^{n-j-1} T_\lambda\psi, T_\lambda\psi\rangle \\
&\quad + \langle T_\lambda\psi, (\mathcal{N}+5)^j [\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)] (\mathcal{N}+5)^{n-j-1} T_\lambda\psi\rangle \Big| \\
&= \Big| \frac{1}{2} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} \sum_{j=0}^{n-1} \langle T_\lambda\psi, (\mathcal{N}+5)^j [\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)] (\mathcal{N}+5)^{n-j-1} T_\lambda\psi\rangle \\
&\quad + \overline{\langle T_\lambda\psi, (\mathcal{N}+5)^{n-j-1} [\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)] (\mathcal{N}+5)^j T_\lambda\psi\rangle} \Big| \\
&= \Big| \mathrm{Re} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} \sum_{j=0}^{n-1} \langle T_\lambda\psi, (\mathcal{N}+5)^j [\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)] (\mathcal{N}+5)^{n-j-1} T_\lambda\psi\rangle \Big|
\end{aligned}
$$

Since $[\mathcal{N}, c_\alpha^*(k)c_\beta^*(k)] = 4c_\alpha^*(k)c_\beta^*(k)$ we find

$$
= \Big| 4\mathrm{Re} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} \sum_{j=0}^{n-1} \langle T_\lambda\psi, (\mathcal{N}+5)^j c_\alpha^*(k)c_\beta^*(k) (\mathcal{N}+5)^{n-j-1} T_\lambda\psi\rangle \Big|.
$$

To distribute the powers of the number operator equally to both arguments of the inner product, we insert $\mathbb{I} = (\mathcal{N}+1)^{\frac{n}{2}-1-j} (\mathcal{N}+5)^{j+1-\frac{n}{2}}$ between $(\mathcal{N}+5)^j$ and $c_\alpha^*(k)$ and then pull $(\mathcal{N}+1)^{j+1-\frac{n}{2}}$ through $c_\alpha^*(k)c_\beta^*(l)$ to the right, by using (5.29). Thus,

$$
\begin{aligned}
&\Big| \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle T_\lambda\psi, (\mathcal{N}+5)^n T_\lambda\psi\rangle \Big| \\
&= \Big| 4\mathrm{Re} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} \sum_{j=0}^{n-1} \langle T_\lambda\psi, (\mathcal{N}+5)^j (\mathcal{N}+1)^{\frac{n}{2}-1-j} (\mathcal{N}+1)^{j+1-\frac{n}{2}} c_\alpha^*(k)c_\beta^*(k) \\
&\quad \times (\mathcal{N}+5)^{n-j-1} T_\lambda\psi\rangle \Big| = \Big| 4\mathrm{Re} \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta} \sum_{j=0}^{n-1} \langle \xi_j, c_\alpha^*(k)c_\beta^*(k)\tilde{\xi}\rangle \Big|
\end{aligned}
$$

where we have introduced $\xi_j := (\mathcal{N}+1)^{\frac{n}{2}-1-j} (\mathcal{N}+5)^j T_\lambda\psi$ and $\tilde{\xi} := (\mathcal{N}+5)^{\frac{n}{2}} T_\lambda\psi$. By Cauchy–Schwarz

$$
\begin{aligned}
\Big| \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle T_\lambda, (\mathcal{N}+5)^n T_\lambda\psi\rangle \Big| &\leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}| \|c_\beta(k)c_\alpha(k)\xi_j\| \|\tilde{\xi}\| \\
&\leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \Big(\sum_{\alpha,\beta\in\mathcal{I}_k} \Big| K(k)_{\alpha,\beta} \Big|^2 \Big)^{1/2} \Big(\sum_{\alpha,\beta\in\mathcal{I}_k} \|c_\beta(k)c_\alpha(k)\xi_j\|^2 \Big)^{1/2} \|\tilde{\xi}\|
\end{aligned}
$$

and using the first bound from Lemma 5.2 we arrive at

$$\begin{aligned}
&\leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \|K(k)\|_{\mathrm{HS}} \Big(\sum_{\alpha,\beta\in\mathcal{I}_k} \|\mathcal{N}(B_{\mathrm{F}}\cap B_\beta)^{1/2} c_\alpha(k)\xi_j\|^2 \Big)^{1/2} \|\tilde{\xi}\| \\
&= 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \|K(k)\|_{\mathrm{HS}} \Big(\sum_{\alpha\in\mathcal{I}_k} \langle c_\alpha(k)\xi_j, \sum_{\beta\in\mathcal{I}_k} \mathcal{N}(B_{\mathrm{F}}\cap B_\beta) c_\alpha(k)\xi_j \Big)^{1/2} \|\tilde{\xi}\|.
\end{aligned}$$

With the trivial estimate $\sum_{\beta\in\mathcal{I}_k} \mathcal{N}(B_{\mathrm{F}}\cap B_\beta) \leq \mathcal{N}$ we get

$$\begin{aligned}
&\leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \|K(k)\|_{\mathrm{HS}} \Big(\sum_{\alpha\in\mathcal{I}_k} \langle c_\alpha(k)\xi_j, \mathcal{N} c_\alpha(k)\xi_j\rangle \Big)^{1/2} \|\tilde{\xi}\| \\
&\leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \|K(k)\|_{\mathrm{HS}} \Big(\sum_{\alpha\in\mathcal{I}_k} \|(\mathcal{N}+2)^{1/2} c_\alpha(k)\xi_j\|^2 \Big)^{1/2} \|\tilde{\xi}\| \\
&= 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \|K(k)\|_{\mathrm{HS}} \Big(\sum_{\alpha\in\mathcal{I}_k} \|c_\alpha(k)\mathcal{N}^{1/2}\xi_j\|^2 \Big)^{1/2} \|\tilde{\xi}\|
\end{aligned}$$

and, estimating $c_\alpha(k)$ by the first bound from Lemma 5.2,

$$\leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} \sum_{j=0}^{n-1} \|K(k)\|_{\mathrm{HS}} \|\mathcal{N}\xi_j\| \|\tilde{\xi}\| \leq 4 \sum_{k\in\Gamma^{\mathrm{nor}}} n\|K(k)\|_{\mathrm{HS}} \langle T_\lambda\psi, (\mathcal{N}+5)^n T_\lambda\psi\rangle. \tag{5.30}$$

Using Grönwall's Lemma for the differential inequality (5.30), we conclude that

$$\langle T_\lambda\psi, (\mathcal{N}+5)^n T_\lambda\psi\rangle \leq \exp\Big(4n\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} \|K(k)\|_{\mathrm{HS}}\Big) \langle\psi, (\mathcal{N}+5)^n\psi\rangle \leq e^{Cn\lambda} \langle\psi, (\mathcal{N}+5)^n\psi\rangle.$$

In the last inequality we used (5.22), estimating the Hilbert–Schmidt norm by $\hat{V}(k)$ and the assumption on V that $\sum_{k\in\mathbb{Z}^3} \hat{V}(k) < C$. □

Recall that our trial state is defined as $T\Omega$. Since we only need the action of $T^* c_\gamma(l) T$ on the trial state, it turns out that we are only interested in knowing the error term (5.18) for the state Ω. Thus, it is sufficient to find a bound for $\sup_{\tau\in[0,1]} \|(\mathcal{N}+2)^{3/2} T_\tau\Omega\|$. This follows from the previous proposition. We can write $(\mathcal{N}+2)^3 = (\mathcal{N}+1)^3 + 3(\mathcal{N}+1)^2 + 3(\mathcal{N}+1) + 1$. Thus, we find

$$\begin{aligned}
\sup_{\tau\in[0,1]} \|(\mathcal{N}+2)^{3/2} T_\tau\Omega\| \leq& \sup_{\tau\in[0,1]} \langle T_\tau\Omega, (\mathcal{N}+1)^3 T_\tau\Omega\rangle + \sup_{\tau\in[0,1]} \langle T_\tau\Omega, 3(\mathcal{N}+1)^2 T_\tau\Omega\rangle \\
&+ \sup_{\tau\in[0,1]} \langle T_\tau\Omega, 3(\mathcal{N}+1) T_\tau\Omega\rangle + \sup_{\tau\in[0,1]} \langle T_\tau\Omega, T_\tau\Omega\rangle \\
\leq& C\Big[\langle\Omega, (\mathcal{N}+5)^3\Omega\rangle + 3\langle\Omega, (\mathcal{N}+5)^2\Omega\rangle + \langle\Omega, (\mathcal{N}+5)\Omega\rangle + \langle\Omega,\Omega\rangle \Big]
\end{aligned}$$

where we used the estimates in Proposition 5.6. Note that $\mathcal{N}\Omega = 0$ and therefore we have $(\mathcal{N}+5)^n\Omega = 5^n\Omega$ for all $n\in\mathbb{N}$. We conclude that

$$\sup_{\tau\in[0,1]} \|(\mathcal{N}+2)^{3/2} T_\tau\Omega\| \leq C. \tag{5.31}$$

Chapter 6

Evaluating the Energy of the Trial State

The focus of this chapter is to evaluate the energy of the trial state. Each term of the correlation Hamiltonian (4.7) is treated individually, showing first that the terms $\mathcal{E}_1$ and $\mathcal{E}_2$ provide subleading corrections to the correlation energy, as well as the direct and the exchange term. Afterwards, it remains to find the expectation value of the kinetic energy and the main contribution of the interaction energy (4.8).

6.1 Getting Rid of Non-Bosonizable Terms

Let us start by showing that the contribution of the two terms $\mathcal{E}_1$ and $\mathcal{E}_2$ defined in (4.4) and (4.5) are negligible if the number of particles tends to infinity. Recall the CAR (2.4)

$$\{a(f), a^*(g)\} = \langle f, g\rangle.$$

For the proofs in this section we will need

$$\begin{aligned}\langle u_x, u_y\rangle &= \langle \delta(\cdot - x) - \sum_{k\in B_\mathrm{F}} f_k(\cdot)\overline{f_k}(x), \delta(\cdot - y) - \sum_{k\in B_\mathrm{F}} f_k(\cdot)\overline{f_k}(y)\rangle \\ &= \langle \delta(\cdot - x), \delta(\cdot - y)\rangle - \langle \delta(\cdot - x), \sum_{k\in B_\mathrm{F}} f_k(\cdot)\overline{f_k}(y)\rangle - \langle \sum_{k\in B_\mathrm{F}} f_k(\cdot)\overline{f_k}(x), \delta(\cdot - y)\rangle \\ &+ \sum_{k_1,k_2\in B_\mathrm{F}} f_{k_1}(x)\overline{f_{k_2}}(y)\langle f_{k_1}, f_{k_2}\rangle = \delta(x-y) - \sum_{k\in B_\mathrm{F}} f_k(x)\overline{f_k}(y) = u(x,y).\end{aligned} \tag{6.1}$$

The lemma below shows that the contribution of $\mathcal{E}_1$ in the state ξ defined in (5.13) is small compared with the desired error of order $o(\hbar)$. The approach is to write $\mathcal{E}_1$ as the second quantization of an operator and using the bounds stated in Section 2.2.

Lemma 6.1 (Non-Bosonizable Interaction Terms)**.** *Let $\mathcal{E}_1(x,y)$ be defined as in* (4.4)*. Let ξ be the trial state defined as in* (5.13)*. Then we have*

$$\left|\langle \xi, \frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3} \mathrm{d}x\mathrm{d}y V(x-y)\mathcal{E}_1(x,y)\xi\rangle\right| \leq CN^{-1}.$$

Proof. We are going to show that for all $\psi \in \mathcal{F}$ we have

$$\Big|\langle\psi, \frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3} \mathrm{d}x\mathrm{d}y V(x-y)\mathcal{E}_1(x,y)\psi\rangle\Big| \leq \frac{2}{N}\sum_{k\in\mathbb{Z}^3}|\hat{V}(k)|\langle\psi,(\mathcal{N}+1)^2\psi\rangle. \tag{6.2}$$

The final claim follows from Proposition 5.6 and the assumption that $\sum_{k\in\mathbb{Z}^3}\hat{V}(k) < C$. To prove (6.2), we rewrite the first term on the r.h.s. of (4.4) by using (6.1):

$$\begin{aligned}
&\frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3} \mathrm{d}x\mathrm{d}y V(x-y)a^*(u_x)a^*(u_y)a(u_y)a(u_x)\\
=&\frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3} \mathrm{d}x\mathrm{d}y V(x-y)\Big(a^*(u_x)a(u_x)a^*(u_y)a(u_y) - a^*(u_x)\langle u_x,u_y\rangle a(u_y)\Big)\\
=&\frac{1}{2N}\sum_{k\in\mathbb{Z}^3}\hat{V}(k)\Big(\int_{\mathbb{T}^3\times\mathbb{T}^3} \mathrm{d}x\mathrm{d}y a^*(u_x)e^{ikx}a(u_x)a^*(u_y)e^{-iky}a(u_y)\\
&- a^*(u_x)e^{ikx}\langle u_x,u_y\rangle e^{-iky}a(u_y)\Big)\\
=&\frac{1}{2N}\sum_{k\in\mathbb{Z}^3}\hat{V}(k)\Big(\mathrm{d}\Gamma(ue^{ikx}u)\mathrm{d}\Gamma(ue^{-ikx}u) - \mathrm{d}\Gamma(ue^{ikx}ue^{-ikx}u)\Big).
\end{aligned}\tag{6.3}$$

Recall Lemma 2.6, stating that for any bounded one-particle operator A and any $\psi\in\mathcal{F}$ we have $\|\mathrm{d}\Gamma(A)\psi\| \leq \|A\|_{\mathrm{op}}\|\mathcal{N}\psi\|$ and $|\langle\psi,\mathrm{d}\Gamma(A)\psi\rangle \leq \|A\|_{\mathrm{op}}\langle\psi,\mathcal{N}\psi\rangle$. Using $\|u\|_{\mathrm{op}}\leq 1$, we find

$$\Big|\langle\psi,\frac{1}{2N}\sum_{k\in\mathbb{Z}^3}\hat{V}(k)\mathrm{d}\Gamma(ue^{ikx}u)\mathrm{d}\Gamma(u^{-ikx}u)\psi\rangle\Big| \leq \frac{1}{2N}\sum_{k\in\mathbb{Z}^3}|\hat{V}(k)|\|\mathcal{N}\xi\|^2.$$

The second summand in (6.3) can be estimated in the same way. The same holds true for the other two terms in (4.4). □

In addition, we need to consider the second error term $\mathcal{E}_2$, defined in (4.5). It turns out that this term vanishes in our trial state ξ.

Lemma 6.2 (Interaction Terms of Wrong Parity)**.** *Let $\mathcal{E}_2(x,y)$ be defined as in* (4.5)*. Let ξ be the trial state defined in* (5.13)*. Then we have*

$$\Big\langle\xi,\frac{1}{2N}\int_{\mathbb{T}^3\times\mathbb{T}^3}\mathrm{d}x\mathrm{d}y V(x-y)\big(\mathcal{E}_2(x,y)+\mathrm{h.c.}\big)\xi\Big\rangle = 0.$$

Proof. Since terms in $\mathcal{E}_2(x,y)$ create exactly two fermions, we have

$$i^{\mathcal{N}}\mathcal{E}_2(x,y) = \mathcal{E}_2(x,y)i^{\mathcal{N}+2} = -\mathcal{E}_2(x,y)i^{\mathcal{N}}.$$

The operator B, defined in (5.17), creates or annihilates exactly four particles at a time. Therefore, it holds $[i^{\mathcal{N}},B]=0$. This implies that $Ti^{\mathcal{N}} = i^{\mathcal{N}}T$. Using $i^{\mathcal{N}}\Omega=\Omega$, we find

$$\begin{aligned}
\langle T\Omega,\mathcal{E}_2T\Omega\rangle &= \langle T\Omega,\mathcal{E}_2Ti^{\mathcal{N}}\Omega\rangle = -\langle T\Omega,i^{\mathcal{N}}\mathcal{E}_2T\Omega\rangle = -\langle(-i)^{\mathcal{N}}T\Omega,\mathcal{E}_2T\Omega\rangle\\
&= -\langle T(-i)^{\mathcal{N}}\Omega,\mathcal{E}_2T\Omega\rangle = -\langle T\Omega,\mathcal{E}_2T\Omega\rangle,
\end{aligned}$$

which thus vanishes. □

6.2 Estimating Direct and Exchange Operator

The next step is to control the energies of $\mathrm{d}\Gamma(uhu - \overline{v}\overline{h}v)$ coming from the direct term $(2\pi)^3\hat{V}(0)$ and from the exchange operator X. Recall that

$$h = -\frac{\hbar^2\Delta}{2} + (2\pi)^3\hat{V}(0) + X$$

where X has the integral kernel $X(x,y) = -N^{-1}V(x-y)\omega_{\mathrm{pw}}(x,y)$. The contribution of the constant direct term $(2\pi)^3\hat{V}(0)$ can be rewritten as

$$(2\pi)^3\hat{V}(0)\mathrm{d}\Gamma(u^2 - \overline{v}v) = (2\pi)^3\hat{V}(0)\mathrm{d}\Gamma(\mathbb{I} - 2\omega_{\mathrm{pw}}) = (2\pi)^3\hat{V}(0)(\mathcal{N}_{\mathrm{p}} - \mathcal{N}_{\mathrm{h}})$$

which vanishes on ξ by Lemma 5.3. The next lemma shows that the contribution of the exchange term X to the expectation $\langle\xi, \mathcal{H}_{\mathrm{corr}}\xi\rangle$ is negligible for $N \to \infty$.

Lemma 6.3 (Bound for the Exchange Term)**.** *Let ξ be the trial state defined as in* (5.13)*. Then, we have*

$$|\langle\xi, \mathrm{d}\Gamma(uXu - \overline{v}\overline{X}v)\xi\rangle| \leq CN^{-1}.$$

Proof. Notice that

$$\omega_{\mathrm{pw}}(x,y) = \frac{1}{(2\pi)^3}\sum_{h\in B_{\mathrm{F}}} e^{ih\cdot(x-y)} =: f(x-y).$$

Thus, X is translation invariant, and hence

$$\|X\|_{\mathrm{op}} = N^{-1}\|\widehat{Vf}\|_{L^\infty} \leq N^{-1}\|\hat{f}\|_{L^\infty}\sum_{k\in\mathbb{Z}^3}|\hat{V}(k)| \leq CN^{-1}.$$

Using that $\|u\|_{\mathrm{op}} = 1 = \|v\|_{\mathrm{op}}$, we get, by Proposition 2.6 and 5.6,

$$|\langle\xi, \mathrm{d}\Gamma(uXu - \overline{v}\overline{X}v)\xi\rangle| \leq \|uXu - \overline{v}\overline{X}v\|_{\mathrm{op}}\langle\xi, \mathcal{N}\xi\rangle \leq CN^{-1}.$$

□

6.3 Expectation Value of the Kinetic Energy

The last term of the one-particle Hartree–Fock Hamiltonian h is the kinetic part. In this section we determine the kinetic energy in the trial stat ξ, as defined in (5.13). We start by linearizing in momentum space

$$\begin{aligned}
-\frac{\hbar^2}{2}\langle\xi, \mathrm{d}\Gamma(u\Delta u - \overline{v}\Delta v)\xi\rangle &= \frac{\hbar^2}{2}\langle\xi, \Big[\sum_{p\in B_{\mathrm{F}}^{\mathrm{c}}} p^2 a_p^* a_p - \sum_{h\in B_{\mathrm{F}}} h^2 a_h^* a_h\Big]\xi\rangle \\
&= \frac{\hbar^2}{2}\langle\xi, \sum_{\alpha=1}^{M}\Big[\sum_{p\in B_{\mathrm{F}}^{\mathrm{c}}\cap B_\alpha}\big((p-\omega_\alpha)^2 + 2p\cdot\omega_\alpha - \omega_\alpha^2\big)a_p^* a_p \\
&\quad - \sum_{h\in B_{\mathrm{F}}\cap B_\alpha}\big((h-\omega_\alpha)^2 + 2h\cdot\omega_\alpha - \omega_\alpha^2\big)a_h^* a_h\Big]\xi\rangle.
\end{aligned}$$

We used that momenta p and h, that lie in the corridors or that are more than a distance N^μ away from the Fermi surface, have disappeared from the sums because such modes are never occupied in the trial state, i.e. $a_p\xi = 0$ and $a_h\xi = 0$. So we can restrict the sum over all possible modes in the patches B_α. Additionally, with Lemma 5.3 we have

$$\langle \xi, \sum_{\alpha=1}^{M} \Big[\sum_{p\in B_{\mathrm{F}}^c \cap B_\alpha} \omega_\alpha^2 a_p^* a_p - \sum_{h\in B_{\mathrm{F}}\cap B_\alpha} \omega_\alpha^2 a_h^* a_h \Big] \xi \rangle = k_{\mathrm{F}}^2 \langle \xi, [\mathcal{N}_p - \mathcal{N}_h]\xi\rangle = 0$$

where we used that $|\omega_\alpha| = k_{\mathrm{F}}$ for all α. Next we want to estimate $(p-\omega)^2$ and $(h-\omega_\alpha)^2$. For that, recall that the diameter of the patch on the Fermi surface is bounded by $C\sqrt{N^{2/3}/M}$. Therefore, the diameter of the patches is also bounded by $C\sqrt{N^{2/3}/M}$ (the diameter of the patch on the Fermi surface is large compared to its thickness of order N^μ since we have $\mu < 1/6 - \varepsilon/2$). Hence,

$$-\frac{\hbar^2}{2}\langle \xi, \mathrm{d}\Gamma(u\Delta u - \overline{v}\Delta v)\xi\rangle = \langle \xi, \mathbb{H}_{\mathrm{kin}}\xi\rangle + \mathfrak{E}_{\mathrm{lin}}$$

where we introduced

$$\mathbb{H}_{\mathrm{kin}} := \hbar^2 \sum_{\alpha=1}^{M} \Big[\sum_{p\in B_{\mathrm{F}}^c\cap B_\alpha} p\cdot\omega_\alpha a_p^* a_p - \sum_{h\in B_{\mathrm{F}}\cap B_\alpha} h\cdot\omega_\alpha a_h^* a_h \Big]$$

and where the error $\mathfrak{E}_{\mathrm{lin}}$ is bounded by

$$\begin{aligned} |\mathfrak{E}_{\mathrm{lin}}| &= \Big| \frac{\hbar^2}{2}\langle \xi, \sum_{\alpha=1}^{M} \Big[\sum_{p\in B_{\mathrm{F}}^c\cap B_\alpha} (p-\omega_\alpha)^2 a_p^* a_p - \sum_{h\in B_{\mathrm{F}}\cap B_\alpha} (h-\omega_\alpha)^2 a_h^* a_h \Big]\xi\rangle \Big| \\ &\leq C\frac{\hbar^2}{2}\frac{N^{2/3}}{M}\langle \xi, \mathcal{N}\xi\rangle \leq \frac{C}{M} \end{aligned}$$

where we used Proposition 5.6 to bound the expectation value of the number operator and $\hbar = N^{-1/3}$.

We need the following lemma to compute the expectation of the linearized kinetic energy operator $\mathbb{H}_{\mathrm{kin}}$, making a statement about the commutator of the linearized kinetic energy operator $\mathbb{H}_{\mathrm{kin}}$ and the creation operator $c_\alpha^*(k)$.

Lemma 6.4 (Kinetic Energy of Particle–Hole Pairs)**.** *For all $k \in \Gamma^{\mathrm{nor}}$ and all $\alpha \in \mathcal{I}_k$ we have*

$$[\mathbb{H}_{\mathrm{kin}}, c_\alpha^*(k)] = \hbar^2 |k\cdot\omega_\alpha| c_\alpha^*(k).$$

Proof. We distinguish the two cases $k\cdot\omega_\alpha > 0$ and $k\cdot\omega_\alpha < 0$. First let $\alpha \in \mathcal{I}_k$ with

$k \cdot \omega_\alpha > 0$. Using CAR, we calculate

$$
\begin{aligned}
[\mathbb{H}_{\mathrm{kin}}, c_\alpha^*(k)] = [\mathbb{H}_{\mathrm{kin}}, b_{\alpha,k}^*] &= [\mathbb{H}_{\mathrm{kin}}, \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in B_{\mathrm{F}}^c \cap B_\alpha \\ h \in B_{\mathrm{F}} \cap B_\alpha}} \delta_{p-h,k} a_p^* a_h^*] \\
&= \hbar^2 \sum_{\beta=1}^{M} \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in B_{\mathrm{F}}^c \cap B_\alpha \\ h \in B_{\mathrm{F}} \cap B_\alpha}} \delta_{p-h,k} \sum_{\tilde{p} \in B_{\mathrm{F}}^c \cap B_\beta} \tilde{p} \cdot \omega_\beta [a_{\tilde{p}}^* a_{\tilde{p}}, a_p^* a_h^*] \\
&\quad - \hbar^2 \sum_{\beta=1}^{M} \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in B_{\mathrm{F}}^c \cap B_\alpha \\ h \in B_{\mathrm{F}} \cap B_\alpha}} \delta_{p-h,k} \sum_{\tilde{h} \in B_{\mathrm{F}} \cap B_\beta} \tilde{h} \cdot \omega_\beta [a_{\tilde{h}}^* a_{\tilde{h}}, a_p^* a_h^*] \\
&= \hbar^2 \sum_{\beta=1}^{M} \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in B_{\mathrm{F}}^c \cap B_\alpha \\ h \in B_{\mathrm{F}} \cap B_\alpha}} \delta_{p-h,k} \Big(\sum_{\tilde{p} \in B_{\mathrm{F}}^c \cap B_\beta} \tilde{p} \cdot \omega_\beta \delta_{p,\tilde{p}} - \sum_{\tilde{h} \in B_{\mathrm{F}} \cap B_\beta} \tilde{h} \cdot \omega_\beta \delta_{h,\tilde{h}} \Big) a_p^* a_h^*.
\end{aligned}
$$

The Kronecker deltas $\delta_{p,\tilde{p}}$ and $\delta_{h,\tilde{h}}$ imply $\beta = \alpha$, thus we get

$$
= \hbar^2 \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in B_{\mathrm{F}}^c \cap B_\alpha \\ h \in B_{\mathrm{F}} \cap B_\alpha}} \delta_{p-h,k} (p-h) \cdot \omega_\alpha a_p^* a_h^* = \hbar^2 |k \cdot \omega_\alpha| c_\alpha^*(k).
$$

The absolute value can be introduced since the scalar product is anyway non-negative. For the second case, $\alpha \in \mathcal{I}_k$ with $k \cdot \omega_\alpha < 0$, we have $c_\alpha^*(k) = b_{\alpha,-k}^*$. The calculation proceeds in the same way, but using $(p-h) \cdot \omega_\alpha = (-k) \cdot \omega_\alpha = |k \cdot \omega_\alpha|$ for the last equality. □

Finally, we have established all tools to calculate the kinetic energy of the trial state. Besides the statement of this section we use that T_λ acts approximately as a bosonic Bogoliubov transformation as stated in Proposition 5.4.

Proposition 6.5 (Kinetic Energy)**.** *Let ξ be defined as in* (5.13)*. Then,*

$$
\langle \xi, \mathbb{H}_{\mathrm{kin}} \xi \rangle = \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \mathrm{tr} D(k) \sinh^2(K(k)) + \mathfrak{E}_{\mathrm{kin}},
$$

where $D(k)$ is defined in (5.16) *and the error term is such that $|\mathfrak{E}_{\mathrm{kin}}| \leq C\hbar N^{3\mu}/\mathfrak{n}^2$ with $\mathfrak{n} = N^{1/3-\delta/2} M^{-1/2}$ as in* (4.16)*.*

Proof. We write $T_\lambda = \exp(\lambda B)$, with B as in (5.17), and $\xi = T\Omega$. Hence,

$$
\begin{aligned}
&\langle \xi, \mathbb{H}_{\mathrm{kin}} \xi \rangle \\
&= \int_0^1 \mathrm{d}\lambda \langle \Omega, T_\lambda^* [\mathbb{H}_{\mathrm{kin}}, B] T_\lambda \Omega \rangle \\
&= \int_0^1 \mathrm{d}\lambda \langle \Omega, T_\lambda^* \Big[\mathbb{H}_{\mathrm{kin}}, \sum_{k \in \Gamma^{\mathrm{nor}}} \frac{1}{2} \sum_{\alpha,\beta \in \mathcal{I}_k} K(k)_{\alpha,\beta} c_\alpha^*(k) c_\beta^* - \mathrm{h.c.} \Big] T_\lambda \Omega \rangle \\
&= \mathrm{Re} \int_0^1 \mathrm{d}\lambda \sum_{k \in \Gamma^{\mathrm{nor}}} \sum_{\alpha,\beta \in \mathcal{I}_k} K(k)_{\alpha,\beta} \langle \Omega, T_\lambda^* \big([\mathbb{H}_{\mathrm{kin}}, c_\alpha^*(k)] c_\beta^*(k) + c_\alpha^*(k) [\mathbb{H}_{\mathrm{kin}}, c_\beta^*(k)] \big) T_\lambda \Omega \rangle.
\end{aligned}
$$

With Lemma 6.4 we get

$$\langle \xi, \mathbb{H}_{\mathrm{kin}} \xi \rangle = \mathrm{Re} \int_0^1 \mathrm{d}\lambda \sum_{k \in \Gamma^{\mathrm{nor}}} \hbar^2 \sum_{\alpha,\beta \in \mathcal{I}_k} K(k)_{\alpha,\beta} (|k \cdot \omega_\alpha| + |k \cdot \omega_\beta|) \langle \Omega, T_\lambda^* c_\alpha^*(k) c_\beta^*(k) T_\lambda \Omega \rangle.$$

Recall that $|k \cdot \omega_\alpha| = |k| \kappa \hbar^{-1} u_\alpha(k)^2$ with $u_\alpha(k)$ defined in (5.12). Using Proposition 5.4 yields

$$\begin{aligned}
\langle \xi, \mathbb{H}_{\mathrm{kin}} \xi \rangle =& \mathrm{Re} \int_0^1 \mathrm{d}\lambda \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \hbar \kappa \sum_{\alpha,\beta \in \mathcal{I}_k} K(k)_{\alpha,\beta} \big(u_\alpha(k)^2 + u_\beta(k)^2 \big) \\
& \times \langle \Omega, \Big(\sum_{\delta \in \mathcal{I}_k} \cosh(\lambda K(k))_{\alpha,\delta} c_\delta^*(k) + \sum_{\delta \in \mathcal{I}_k} \sinh(\lambda K(k))_{\alpha,\delta} c_\delta(k) + \mathfrak{E}_\alpha^*(\lambda, k) \Big) \\
& \times \Big(\sum_{\gamma \in \mathcal{I}_k} \cosh(\lambda K(k))_{\beta,\gamma} c_\gamma^*(k) + \sum_{\gamma \in \mathcal{I}_k} \sinh(\lambda K(k))_{\beta,\gamma} c_\gamma(k) + \mathfrak{E}_\beta^*(\lambda, k) \Big) \Omega \rangle.
\end{aligned}$$

By using $c_\delta(k)\Omega = 0$ and $\langle \Omega, c_\delta(k) c_\gamma^*(k) \Omega \rangle = \delta_{\delta,\gamma}$, we get

$$\begin{aligned}
\langle \xi, \mathbb{H}_{\mathrm{kin}} \xi \rangle &= \mathrm{Re} \int_0^1 \mathrm{d}\lambda \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \hbar \kappa \sum_{\alpha,\beta \in \mathcal{I}_k} K(k)_{\alpha,\beta} \big(u_\alpha(k)^2 + u_\beta(k)^2 \big) \\
&\quad \times \sum_{\delta \in \mathcal{I}_k} \sinh(\lambda K(k))_{\alpha,\delta} \sum_{\gamma \in \mathcal{I}_k} \cosh(\lambda K(k))_{\beta,\gamma} \delta_{\delta,\gamma} + \mathfrak{E}_{\mathrm{kin}} \\
&= \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \hbar \kappa \sum_{\alpha \in \mathcal{I}_k} u_\alpha(k)^2 \int_0^1 \mathrm{d}\lambda \Big(\sinh(2\lambda K(k)) K(k) \Big)_{\alpha,\alpha} + \mathfrak{E}_{\mathrm{kin}} \qquad (6.4)
\end{aligned}$$

where we defined

$$\begin{aligned}
\mathfrak{E}_{\mathrm{kin}} :=& \mathrm{Re} \int_0^1 \mathrm{d}\lambda \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \hbar \kappa \sum_{\alpha,\beta \in \mathcal{I}_k} K(k)_{\alpha,\beta} \big(u_\alpha(k)^2 + u_\beta(k)^2 \big) \\
& \times \Big(\langle \Omega, \mathfrak{E}_\alpha^*(\lambda, k) \mathfrak{E}_\beta^*(\lambda, k) \Omega \rangle + \sum_{\delta \in \mathcal{I}_k} \sinh(\lambda K(k))_{\alpha,\delta} \langle \Omega, c_\delta(k) \mathfrak{E}_\beta^*(\lambda, k) \Omega \rangle \\
& + \sum_{\gamma \in \mathcal{I}_k} \cosh(\lambda K(k))_{\beta,\gamma} \langle \Omega, \mathfrak{E}_\alpha^*(\lambda, k) c_\gamma^*(k) \Omega \rangle \Big) \\
=:& \, \mathfrak{E}_{\mathrm{kin}}^{(1)} + \mathfrak{E}_{\mathrm{kin}}^{(2)} + \mathfrak{E}_{\mathrm{kin}}^{(3)}. \qquad (6.5)
\end{aligned}$$

Notice that for any $a \in \mathbb{R}$

$$\begin{aligned}
\int_0^1 \mathrm{d}\lambda \sinh(2\lambda a) a &= \frac{1}{2} \big[\cosh(2a) - \cosh(0) \big] \\
&= \frac{1}{2} \big[\cosh^2(a) + \sinh^2(a) - 1 \big] = \sinh^2(a) \qquad (6.6)
\end{aligned}$$

where we used the equation $\cosh^2(a) - \sinh^2(a) = 1$. With (6.6) we can compute the integral in (6.4). We find

$$\langle \xi, \mathbb{H}_{\mathrm{kin}} \xi \rangle = \hbar \kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \mathrm{tr} D(k) \sinh^2(K(k)) + \mathfrak{E}_{\mathrm{kin}}.$$

To estimate the error term $\mathfrak{E}_{\mathrm{kin}}$ we start by bounding the first error term of (6.5). Using $u_\alpha(k)^2 = |\hat{k}\cdot\hat{\omega}_a| \leq 1$ and Cauchy–Schwarz, we get

$$\begin{aligned}
|\mathfrak{E}_{\mathrm{kin}}^{(1)}| &\leq \Big| \int_0^1 \mathrm{d}\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} |k|\hbar\kappa \sum_{\alpha,\beta\in\mathcal{I}_k} K(k)_{\alpha,\beta}\big(u_\alpha(k)^2 + u_\beta(k)^2\big)\langle\Omega, \mathfrak{E}_\alpha^*(\lambda,k)\mathfrak{E}_\beta^*(\lambda,k)\Omega\rangle\Big| \\
&\leq 2\int_0^1 \mathrm{d}\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} |k|\hbar\kappa \sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}| \|\mathfrak{E}_\alpha(\lambda,k)\Omega\| \|\mathfrak{E}_\beta^*(\lambda,k)\Omega\| \\
&\leq 2\int_0^1 \mathrm{d}\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} |k|\hbar\kappa \Big[\sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}|^2\Big]^{1/2} \Big[\sum_{\alpha\in\mathcal{I}_k} \|\mathfrak{E}_\alpha(\lambda,k)\Omega\|^2\Big]^{1/2} \\
&\quad \times \Big[\sum_{\beta\in\mathcal{I}_k} \|\mathfrak{E}_\beta^*(\lambda,k)\Omega\|^2\Big]^{1/2}.
\end{aligned}$$

With the bound (5.18) we find

$$|\mathfrak{E}_{\mathrm{kin}}^{(1)}| \leq \frac{C\hbar}{\mathfrak{n}^4} N^{2\mu} \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \|K(k)\|_{\mathrm{HS}} e^{2\|K(k)\|_{\mathrm{HS}}} \sup_{\lambda\in[0,1]} \langle T_\lambda\Omega, (\mathcal{N}+2)^3 T_\lambda\Omega\rangle \Big[\sum_{l\in\Gamma^{\mathrm{nor}}} \|K(l)\|_{\mathrm{HS}}\Big]^2.$$

Recall that $|k| \leq N^\mu$. With Proposition 5.6 we can control the term containing the supremum and with Lemma 5.5 we can control the terms containing $\|K(k)\|_{\mathrm{HS}}$. We conclude that $|\mathfrak{E}_{\mathrm{kin}}^{(1)}| \leq \frac{C\hbar}{\mathfrak{n}^4} N^{3\mu}$. The third error term $\mathfrak{E}_{\mathfrak{tin}}^{(3)}$ can be controlled similarly. Using Lemma 5.2 yields

$$\begin{aligned}
|\mathfrak{E}_{\mathrm{kin}}^{(3)}| &\leq C\hbar \int_0^1 \mathrm{d}\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}| \Big| \sum_{\gamma\in\mathcal{I}_k} \cosh(\lambda K(k))_{\beta,\gamma} \langle \mathfrak{E}_\alpha(\lambda,k)\Omega, c_\gamma^*(k)\Omega\rangle\Big| \\
&\leq C\hbar \int_0^1 \mathrm{d}\lambda \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}| \Big\| \sum_{\gamma\in\mathcal{I}_k} \cosh(\lambda K(k))_{\beta,\gamma} c_\gamma^*(k)\Omega\Big\| \|\mathfrak{E}_\alpha(\lambda,k)\Omega\| \\
&\leq C\hbar \int_0^1 \mathrm{d}\lambda \|(\mathcal{N}+1)^{1/2}\Omega\| \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}| \Big[\sum_{\gamma\in\mathcal{I}_k} |\cosh(\lambda K(k))_{\beta,\gamma}|^2\Big]^{1/2} \\
&\quad \times \|\mathfrak{E}_\alpha(\lambda,k)\Omega\|
\end{aligned}$$

which can be estimated by

$$\begin{aligned}
&\leq C\hbar \int_0^1 \mathrm{d}\lambda \|(\mathcal{N}+1)^{1/2}\Omega\| \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \Big[\sum_{\beta,\gamma\in\mathcal{I}_k} |\cosh(\lambda K(k))_{\beta,\gamma}|^2\Big]^{1/2} \Big[\sum_{\alpha,\beta\in\mathcal{I}_k} |K(k)_{\alpha,\beta}|^2\Big]^{1/2} \\
&\quad \times \Big[\sum_{\alpha\in\mathcal{I}_k} \|\mathfrak{E}_\alpha(\lambda,k)\Omega\|^2\Big]^{1/2} \\
&\leq C\hbar \int_0^1 \mathrm{d}\lambda \|(\mathcal{N}+1)^{1/2}\Omega\| \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \|\cosh(\lambda K(k))\|_{\mathrm{HS}} \|K(k)\|_{\mathrm{HS}} \sup_{\tau\in[0,\lambda]} \|(\mathcal{N}+2)^{3/2} T_\tau\Omega\| \\
&\quad \times \frac{N^\mu}{\mathfrak{n}^2} e^{\lambda\|K(k)\|_{\mathrm{HS}}} \sum_{l\in\Gamma^{\mathrm{nor}}} \|K(l)\|_{\mathrm{HS}}
\end{aligned}$$

by using Cauchy–Schwarz and by Proposition 5.4. Further, we get

$$\begin{aligned}
&\leq \frac{C\hbar}{\mathfrak{n}^2} N^{\mu} \|(\mathcal{N}+1)^{1/2}\Omega\| \sup_{\lambda\in[0,1]} \|(\mathcal{N}+2)^{2/3} T_\lambda \Omega\| \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \|K(k)\|_{\mathrm{HS}} e^{\|K(k)\|_{\mathrm{HS}}} \\
&\quad \times \int_0^1 \mathrm{d}\lambda \|\cosh(\lambda K(k))\|_{\mathrm{HS}} \sum_{l\in\Gamma^{\mathrm{nor}}} \|K(l)\|_{\mathrm{HS}} \\
&\leq \frac{C\hbar}{\mathfrak{n}^2} N^{\mu} \|(\mathcal{N}+1)^{1/2}\Omega\| \sup_{\lambda\in[0,1]} \|(\mathcal{N}+2)^{2/3} T_\lambda \Omega\| \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \|K(k)\|_{\mathrm{HS}} e^{2\|K(k)\|_{\mathrm{HS}}} \\
&\quad \times \sum_{l\in\Gamma^{\mathrm{nor}}} \|K(l)\|_{\mathrm{HS}} \leq \frac{C\hbar}{\mathfrak{n}^2} N^{3\mu}.
\end{aligned}$$

The second error term $\mathfrak{E}_{\mathrm{kin}}^{(2)}$ can be estimated in the same way and we conclude that $|\mathfrak{E}_{\mathrm{kin}}| \leq \frac{C\hbar}{\mathfrak{n}^2} N^{2\mu}$. □

6.4 Expectation Value of the Interaction Energy

We are left with calculating the main contribution of the interaction energy Q_N^{B}. This is the task of the proposition in this section. We use that modes in the corridor or in patches near the equator give small contribution to the energy. By the characterization of T_λ we find the demanded expression.

Proposition 6.6 (Interaction Energy)**.** *Let ξ be the trial state defined as in* (5.13)*, and let Q_N^{B} be given by* (4.8)*. Then*

$$\begin{aligned}
\langle \xi, Q_N^{\mathrm{B}} \xi \rangle = \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \mathrm{tr}\Big(W(k) \sinh^2(K(k)) + \tilde{W}(k) \sinh(K(k)) \cosh(K(k)) \Big) \\
+ \mathfrak{E}_{\mathrm{int}} + \mathcal{O}(\hbar N^{-\delta/2+\mu})
\end{aligned}$$

where $W(k)$ and $\tilde{W}(k)$ are defined in (5.16)*. The error is bounded by $|\mathfrak{E}_{\mathrm{int}}| \leq C\hbar N^{3\mu}/\mathfrak{n}^2$, with $\mathfrak{n} = N^{1/3-\delta/2} M^{-1/2}$ as in* (4.16)*.*

Proof. We remind you of the decomposition of the b_k-operators by their patch decomposition (4.14),

$$\tilde{b}_k = \sum_{\alpha\in\mathcal{I}_k^+} \tilde{b}_{\alpha,k} + \mathfrak{r}_k. \tag{6.7}$$

and that the error terms $\mathfrak{r}_k$ collect modes in the corridors and close to the equator. We can write

$$\mathfrak{r}_k = \tilde{\mathfrak{r}}_k + \sum_{\alpha\notin\mathcal{I}_k} \tilde{b}_{\alpha,k}, \tag{6.8}$$

where $\tilde{\mathfrak{r}}_k$ is a linear combination of product $a_h a_p$ such that at least one of the two momenta is in the corridor B_{corri}, and the second term collects the contributions coming from the patches close to the equator. To prove the proposition we are going to show that the contribution of $\mathfrak{r}_k$ (the contribution of the corridor and of patches near the equator) is negligible. Afterwards, we will show that the contributions of the $\tilde{b}_{\alpha,k}$-operators, with

$\alpha \in \mathcal{I}_k$, produce the desired expression.

Contribution of the Corridors. We expect that there is no contribution of the error term $\tilde{\mathfrak{r}}_k$. Indeed, the operator B, used to define $T = e^B$, does not contain any mode $q \in B_{\text{corri}}$. This implies that $\tilde{\mathfrak{r}}_k \xi = 0$ since at least one of the two momenta p and h appearing in $\tilde{\mathfrak{r}}_k$ is in the corridor B_{corri}. Plugging the Decomposition (6.7) into Q_N^{B} from (4.11) and taking the expectation value on ξ, we realize that all terms containing at least one error operator $\tilde{\mathfrak{r}}_k^\natural$ are zero because there is at least one error operator $\tilde{\mathfrak{r}}_k$ acting directly on $T\Omega$.

Contribution of Patches near the equator. We claim that the contribution to $\langle \xi, Q_N^{\mathrm{B}} \xi \rangle$ coming form patches $\beta \notin \mathcal{I}_k$ (patches β in the collar where $|\hat{k} \cdot \hat{\omega}_\beta| < N^{-\delta}$) is subleading as $N \to \infty$. The number of particle–hole pairs in this collar and at most a distance N^μ away from the surface is an upper bound for $\sum_{\beta \notin \mathcal{I}_k} n_{\beta,k}^2$. This is because additionally, we allow momenta to be in the corridors. The idea is to show that the number of particle–hole pairs in the collar, containing all such patches, is small. We will estimate the area of the collar followed by using Gauss' classical argument. For the first task we mention that the width of the collar is bounded from above by $Ck_{\mathrm{F}}N^{-\delta}$ and its length is bounded from above by the circumference of the equator Ck_{F}. Thus the surface area of the collar is bounded by $Ck_{\mathrm{F}}^2 N^{-\delta}$. The number of particle–hole pairs related to the collar can be counted by Gauss' classical argument: assign to each lattice point x the cube $[x_1, x_1+1] \times [x_2, x_2+1] \times [x_3, x_3+1]$. Then the number of cubes belonging to lattice points near the collar is bounded by the Lebesgue measure of the collar "fattened" to a thickness N^μ:

$$\sum_{\beta \notin \mathcal{I}_k} n_{\beta,k}^2 \leq Ck_{\mathrm{F}}^2 N^{-\delta} \times N^\mu = \mathcal{O}(N^{2/3-\delta+\mu}). \tag{6.9}$$

We can now estimate the contribution of modes close to the equator to $\langle \xi, Q_N^{\mathrm{B}} \xi \rangle$. First consider the term $\frac{1}{2N} \sum_{k \in \Gamma^{\mathrm{nor}}} \hat{V}(k) 2 \tilde{b}_k^* \tilde{b}_k$. We get three contributions from (6.8), namely

$$\begin{aligned}
&\frac{1}{N} \sum_{k \in \Gamma^{\mathrm{nor}}} \hat{V}(k) \sum_{\beta \notin \mathcal{I}_k} \tilde{b}_{\beta,k}^* \sum_{\alpha \in \mathcal{I}_k^+} \tilde{b}_{\alpha,k}, \\
&\frac{1}{N} \sum_{k \in \Gamma^{\mathrm{nor}}} \hat{V}(k) \sum_{\beta \in \mathcal{I}_k^+} \tilde{b}_{\beta,k}^* \sum_{\alpha \notin \mathcal{I}_k} \tilde{b}_{\alpha,k}, \\
&\frac{1}{N} \sum_{k \in \Gamma^{\mathrm{nor}}} \hat{V}(k) \sum_{\beta \notin \mathcal{I}_k} \tilde{b}_{\beta,k}^* \sum_{\alpha \notin \mathcal{I}_k} \tilde{b}_{\alpha,k}.
\end{aligned} \tag{6.10}$$

We give detailed estimate for the first term in the list, the other two terms can be controlled similarly. We use Lemma 5.2. (Notice that in the original lemma the sum is over $\mathcal{I}_k$. Here however the sum is over $\mathcal{I}_k^+$ and over patches not contained in $\mathcal{I}_k$. The proof for these

statement work in the same way as the proof of the original lemma.) We get

$$\begin{aligned}
&\frac{1}{N}\sum_{k\in\Gamma^{\mathrm{nor}}}\Big\langle\xi,\sum_{\beta\notin\mathcal{I}_k}\tilde{b}^*_{\beta,k}\sum_{\alpha\in\mathcal{I}_k^+}\tilde{b}_{\alpha,k}\xi\Big\rangle\\
=&\frac{1}{N}\sum_{k\in\Gamma^{\mathrm{nor}}}\Big\langle\xi,\sum_{\beta\notin\mathcal{I}_k}n_{\beta,k}b^*_{\beta,k}\sum_{\alpha\in\mathcal{I}_k^+}n_{\alpha,k}b_{\alpha,k}\xi\Big\rangle\\
\leq&\frac{1}{N}\sum_{k\in\Gamma^{\mathrm{nor}}}\hat{V}(k)\Big\|\sum_{\beta\notin\mathcal{I}_k}n_{\beta,k}b_{\beta,k}\xi\Big\|\Big\|\sum_{\alpha\in\mathcal{I}_k^+}n_{\alpha,k}b_{\alpha,k}\xi\Big\|\\
\leq&\frac{1}{N}\sum_{k\in\Gamma^{\mathrm{nor}}}\hat{V}(k)\Big(\sum_{\beta\notin\mathcal{I}_k}n^2_{\beta,k}\Big)^{1/2}\|\mathcal{N}^{1/2}\xi\|\Big(\sum_{\alpha\in\mathcal{I}_k^+}n^2_{\alpha,k}\Big)^{1/2}\|\mathcal{N}^{1/2}\xi\|\\
\leq&\frac{1}{N}\sum_{k\in\Gamma^{\mathrm{nor}}}\hat{V}(k)\Big(CN^{2/3-\delta+\mu}\Big)^{1/2}\Big(M\frac{Ck_{\mathrm{F}}^2}{M}N^{\mu}\Big)^{1/2}\langle\xi,\mathcal{N}\xi\rangle=\mathcal{O}(\hbar N^{-\delta/2+\mu})
\end{aligned}$$

where we used (6.9) to estimate the sum over $\beta\notin\mathcal{I}_k$, $n^2_{\alpha,k}\leq CN^{\mu}k_{\mathrm{F}}^2/M$, due to Proposition 4.1, for the sum over $\alpha\in\mathcal{I}_k$, and the bound on the number of fermions $\mathcal{N}$ from Proposition 5.6.
All other terms of (4.11) can be controlled in a similar way (for example using the bound for $b^*_{\alpha,k}$ in Lemma 5.2). We conclude that the contribution to $\langle\xi,Q_N^{\mathrm{B}}\xi\rangle$ coming from modes close to the equator is of order $\mathcal{O}(\hbar N^{-\delta/2+\mu})$.

Approximate Bogoliubov Diagonalization of the Effective Interaction. It remains to compute the contribution of the pairs of $b_{\alpha,k}$-operators collecting modes in the patches away from the equator. By the discussion of the previous paragraph

$$\begin{aligned}
&\langle\xi,Q_N^{\mathrm{B}}\xi\rangle\\
&=\frac{1}{N}\langle\xi,\sum_{k\in\Gamma^{\mathrm{nor}}}\hat{V}(k)\Big(\sum_{\alpha,\beta\in\mathcal{I}_k^+}\tilde{b}^*_{\alpha,k}\tilde{b}_{\beta,k}+\sum_{\alpha,\beta\in\mathcal{I}_k^-}\tilde{b}^*_{\alpha,-k}\tilde{b}_{\beta,-k}+\Big[\sum_{\alpha\in\mathcal{I}_k^+,\beta\in\mathcal{I}_k^-}\tilde{b}^*_{\alpha,k}b^*_{\beta,-k}+\mathrm{h.c.}\Big]\Big)\xi\rangle\\
&\quad+\mathcal{O}(\hbar N^{-\delta/2+\mu})
\end{aligned}$$

where we used that

$$\sum_{\substack{\alpha\in\mathcal{I}_k^+\\ \beta\in\mathcal{I}_k^-}}\tilde{b}^*_{\alpha,k}\tilde{b}^*_{\beta,-k}=\sum_{\substack{\alpha\in\mathcal{I}_k^-\\ \beta\in\mathcal{I}_k^+}}\tilde{b}^*_{\alpha,-k}\tilde{b}^*_{\beta,k}\quad\text{(and the same for the hermite conjugate).}$$

We rewrite the $\tilde{b}^*_{\alpha,k}$ and $\tilde{b}_{\alpha,k}$ in terms of the normalization factors $n_{\alpha,k}=k_{\mathrm{F}}\sqrt{|k|}v_\alpha(k)$ and the operators $c^*_\alpha(k)$ and $c_\alpha(k)$, defined in (5.1). We find

$$\langle\xi,Q_N^{\mathrm{B}}\xi\rangle=\langle\xi,\mathbb{H}_{\mathrm{int}}\xi\rangle+\mathcal{O}(\hbar N^{-\delta/2+\mu}),\qquad\mathbb{H}_{\mathrm{int}}:=\mathbb{H}^{(1)}_{\mathrm{int}}+\mathbb{H}^{(2)}_{\mathrm{int}}+\mathbb{H}^{(3)}_{\mathrm{int}},\tag{6.11}$$

where, recalling that $g(k) = \kappa\hat{V}(k)$,

$$\mathbb{H}^{(1)}_{\rm int} := \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) c^*_\alpha(k) c_\beta(k),$$

$$\mathbb{H}^{(2)}_{\rm int} := \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^-_k} v_\alpha(k) v_\beta(k) c^*_\alpha(k) c_\beta(k),$$

$$\mathbb{H}^{(3)}_{\rm int} := \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha\in\mathcal{I}^+_k} \sum_{\beta\in\mathcal{I}^-_k} v_\alpha(k) v_\beta(k) c^*_\alpha(k) c^*_\beta(k) + \text{h.c.}$$

We evaluate the expectation values $\langle \xi, \mathbb{H}^{(i)}_{\rm int}\xi\rangle$ for $i = 1,2,3$, with $\xi = T\Omega$, using the fact that the T operator behaves as an approximate bosonic Bogoliubov transformation according to Proposition 5.4. With $\langle \Omega, c_\delta(k) c^*_\gamma(k)\Omega\rangle = \delta_{\delta,\gamma}$, we find

$$\begin{aligned}
\langle \xi, \mathbb{H}^{(1)}_{\rm int}\xi\rangle &= \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) \langle \Omega, T^* c^*_\alpha(k) c_\beta(k) T\Omega\rangle \\
&= \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) \langle \Omega, \\
&\quad \times \Big[\sum_{\gamma\in\mathcal{I}_k} \cosh(K(k))_{\gamma,\alpha} c^*_\gamma(k) + \sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} c_\gamma(k) + \mathfrak{E}^*_\alpha(1,k) \Big] \\
&\quad \times \Big[\sum_{\delta\in\mathcal{I}_k} \cosh(K(k))_{\delta,\beta} c_\delta(k) + \sum_{\delta\in\mathcal{I}_k} \sinh(K(k))_{\delta,\beta} c^*_\delta(k) + \mathfrak{E}_\beta(1,k) \Big] \Omega\rangle \\
&= \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) \langle \Omega, \Big[\sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} c_\gamma(k) + \mathfrak{E}^*_\alpha(1,k) \Big] \\
&\quad \times \Big[\sum_{\delta\in\mathcal{I}_k} \sinh(K(k))_{\delta,\beta} c^*_\delta(k) + \mathfrak{E}_\beta(1,k) \Big] \Omega\rangle \\
&= \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) \sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} \sinh(K(k))_{\gamma,\beta} + \mathfrak{E}^{(1)}_{\rm int}
\end{aligned}$$

where the error term is given by

$$\begin{aligned}
\mathfrak{E}^{(1)}_{\rm int} = \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}^+_k} v_\alpha(k) v_\beta(k) \Big[&\sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} \langle \Omega, c_\gamma(k) \mathfrak{E}_\beta(1,k)\Omega\rangle \\
&+ \sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\beta} \langle \Omega, \mathfrak{E}^*_\alpha(1,k) c^*_\gamma(k)\Omega\rangle + \langle \Omega, \mathfrak{E}^*_\alpha(1,k)\mathfrak{E}_\beta(1,k)\Omega\rangle \Big].
\end{aligned}$$

The expectation value $\langle \xi, \mathbb{H}^{(1)}_{\rm int}\xi\rangle$ can be further simplified to

$$\langle \xi, \mathbb{H}^{(1)}_{\rm int}\xi\rangle = \hbar\kappa \sum_{k\in\Gamma^{\rm nor}} |k| \mathrm{tr} W^{++}(k) \sinh^2(K(k)) + \mathfrak{E}^{(1)}_{\rm int}. \tag{6.12}$$

where

$$W^{++}(k)_{\alpha,\beta} = \begin{cases} g(k) v_\alpha(k) v_\beta(k) & \text{for } \alpha,\beta \in \mathcal{I}^+_k \\ 0 & \text{otherwise} \end{cases}.$$

Here, we used that $\mathrm{tr}(ABC) = \sum_l \sum_j \sum_k a_{l,k} b_{k,j} c_{j,l}$ and that the matrices are symmetric. Also using Proposition 5.4 for the second part of the interaction, we get

$$\langle \xi, \mathbb{H}_{\mathrm{int}}^{(2)} \xi \rangle = \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \mathrm{tr} W^{--}(k) \sinh^2(K(k)) + \mathfrak{E}_{\mathrm{int}}^{(2)}, \tag{6.13}$$

where

$$W^{--}(k)_{\alpha,\beta} = \begin{cases} g(k) v_\alpha(k) v_\beta(k) & \text{for } \alpha, \beta \in \mathcal{I}_k^- \\ 0 & \text{otherwise} \end{cases}$$

and

$$\begin{aligned} \mathfrak{E}_{\mathrm{int}}^{(2)} = \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| g(k) \sum_{\alpha,\beta \in \mathcal{I}_k^-} v_\alpha(k) v_\beta(k) \Big[\sum_{\gamma \in \mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} \langle \Omega, c_\gamma(k) \mathfrak{E}_\beta(1,k) \Omega \rangle \\ + \sum_{\gamma \in \mathcal{I}_k} \sinh(K(k))_{\gamma,\beta} \langle \Omega, \mathfrak{E}_\alpha^*(1,k) c_\gamma^*(1,k) \Omega \rangle + \langle \Omega, \mathfrak{E}_\alpha^*(1,k) \mathfrak{E}_\beta(1,k) \Omega \rangle \Big]. \end{aligned}$$

Finally, for the third interaction we find

$$\begin{aligned} \langle \xi, \mathbb{H}_{\mathrm{int}}^{(3)} \xi \rangle &= 2\hbar\kappa \, \mathrm{Re} \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \mathrm{tr} W^{+-}(k) \sinh(K(k)) \cosh(K(k)) + \mathfrak{E}_{\mathrm{int}}^{(3)} \\ &= \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \mathrm{tr} \tilde{W}(k) \sinh(K(k)) \cosh(K(k)) + \mathfrak{E}_{\mathrm{int}}^{(3)}, \end{aligned} \tag{6.14}$$

where

$$W^{+-}(k)_{\alpha,\beta} = \begin{cases} g(k) v_\alpha(k) v_\beta(k) & \text{for } \alpha \in \mathcal{I}_k^+ \text{ and } \beta \in \mathcal{I}_k^- \\ 0 & \text{otherwise} \end{cases}.$$

We used the fact that all terms are real to write the more symmetric expression in terms of $\tilde{W}(k) = W^{+-}(k) + W^{-+}(k)$. The latter $W^{-+}(k)$ is defined by exchanging the role of $\mathcal{I}_k^+$ and $\mathcal{I}_k^-$ in the former. The error term $\mathfrak{E}_{\mathrm{int}}^{(3)}$ is given by

$$\begin{aligned} \mathfrak{E}_{\mathrm{int}}^{(3)} = 2\hbar\kappa \, \mathrm{Re} \sum_{k \in \Gamma^{\mathrm{nor}}} |k| g(k) \sum_{\alpha \in \mathcal{I}_k^+} \sum_{\beta \in \mathcal{I}_k^-} v_\alpha(k) v_\beta(k) \Big[\sum_{\gamma \in \mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} \langle \Omega, c_\gamma(k) \mathfrak{E}_\beta^*(1,k) \Omega \rangle \\ + \sum_{\gamma \in \mathcal{I}_k} \cosh(K(k))_{\gamma,\beta} \langle \Omega, \mathfrak{E}_\alpha^*(1,k) c_\gamma^*(k) \Omega \rangle + \langle \Omega, \mathfrak{E}_\alpha^*(1,k) \mathfrak{E}_\beta^*(1,k) \Omega \rangle \Big]. \end{aligned}$$

Combining the three parts (6.12), (6.13) and (6.14) with (6.11), we conclude that

$$\begin{aligned} \langle \xi, Q_N^{\mathrm{B}} \xi \rangle = \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \mathrm{tr} \Big(W(k) \sinh^2(K(k)) + \tilde{W}(k) \sinh(K(k)) \cosh(K(k)) \Big) + \mathfrak{E}_{\mathrm{int}} \\ + \mathcal{O}(\hbar N^{-\delta/2+\mu}) \end{aligned}$$

with $\mathfrak{E}_{\mathrm{int}} = \mathfrak{E}_{\mathrm{int}}^{(1)} + \mathfrak{E}_{\mathrm{int}}^{(2)} + \mathfrak{E}_{\mathrm{int}}^{(3)}$. We control $\mathfrak{E}_{\mathrm{int}}^{(1)}$ by decomposing it as

$$\begin{aligned} \mathfrak{E}_{\mathrm{int}}^{(1)} &= \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| g(k) \sum_{\alpha,\beta \in \mathcal{I}_k^+} v_\alpha(k) v_\beta(k) \Big[\sum_{\gamma \in \mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} \langle \Omega, c_\gamma(k) \mathfrak{E}_\beta(1,k) \Omega \rangle \\ &\quad + \sum_{\gamma \in \mathcal{I}_k} \sinh(K(k))_{\gamma,\beta} \langle \Omega, \mathfrak{E}_\alpha^*(1,k) c_\gamma^*(k) \Omega \rangle + \langle \Omega, \mathfrak{E}_\alpha^*(1,k) \mathfrak{E}_\beta(1,k) \Omega \Big] \\ &=: \mathfrak{E}_{\mathrm{int}}^{(1,1)} + \mathfrak{E}_{\mathrm{int}}^{(1,2)} + \mathfrak{E}_{\mathrm{int}}^{(1,3)}. \end{aligned}$$

Recall that $u_\alpha(k)^2 = |\hat{k} \cdot \hat{\omega}_\alpha| \leq 1$ and hence, by Proposition 4.1, $v_\alpha(k) \leq \sqrt{C/M} u_\alpha(k) \leq \sqrt{C/M}$. Thus, using Proposition 5.4 and Cauchy–Schwarz (of the form $|\langle x, y\rangle| \leq \|x\| \cdot \|y\|$ and of the form $\sum_{j\in J} a_j \leq (\sum_{j\in J} a_j^2)^{1/2} \cdot |J|^{1/2}$), we find

$$\begin{aligned}
|\mathfrak{E}_{\mathrm{int}}^{(1,3)}| &\leq \Big| \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}_k^+} v_\alpha(k) v_\beta(k) \langle \Omega, \mathfrak{E}_\alpha^*(1,k) \mathfrak{E}_\beta(1,k)\Omega\rangle \Big| \\
&\leq \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k| g(k) \sum_{\alpha\in\mathcal{I}_k^+} \sqrt{\frac{C}{M}} \|\mathfrak{E}_\alpha(1,k)\Omega\| \sum_{\beta\in\mathcal{I}_k^+} \sqrt{\frac{C}{M}} \|\mathfrak{E}_\beta(1,k)\Omega\| \\
&\leq C\hbar \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \hat{V}(k) \sum_{\alpha\in\mathcal{I}_k^+} \|\mathfrak{E}_\alpha(1,k)\Omega\|^2,
\end{aligned}$$

where we used that $|\mathcal{I}_k^+| = I_k \leq M/2$. With (5.18), we get

$$|\mathfrak{E}_{\mathrm{int}}^{(1,3)}| \leq \hbar \frac{C}{\mathfrak{n}^4} N^{2\mu} \sup_{\lambda\in[0,1]} \langle T_\lambda \Omega, (\mathcal{N}+2)^3 T_\lambda \Omega\rangle \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \hat{V}(k) e^{2\|K(k)\|_{\mathrm{HS}}} \Big[\sum_{l\in\Gamma^{\mathrm{nor}}} \|K(l)\|_{\mathrm{HS}} \Big]^2.$$

Lemma 5.5 and Proposition 5.6 imply that $|\mathfrak{E}_{\mathrm{int}}^{(1,3)}| \leq C\frac{\hbar}{\mathfrak{n}^4} N^{3\mu}$. The term $\mathfrak{E}_{\mathrm{int}}^{(1,1)}$ can be controlled similarly, namely,

$$\begin{aligned}
|\mathfrak{E}_{\mathrm{int}}^{(1,1)}| &\leq \Big| \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k| g(k) \sum_{\alpha,\beta\in\mathcal{I}_k^+} v_\alpha(k) v_\beta(k) \sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} \langle \Omega, c_\gamma(k) \mathfrak{E}_\beta(k,1)\Omega\rangle \Big| \\
&\leq \frac{C\hbar}{M} \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \hat{V}(k) \sum_{\alpha,\beta\in\mathcal{I}_k^+} \Big\| \sum_{\gamma\in\mathcal{I}_k} \sinh(K(k))_{\gamma,\alpha} c_\gamma^*(k)\Omega \Big\| \|\mathfrak{E}_\beta(k,1)\Omega\| \\
&\leq \frac{C\hbar}{M} \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \hat{V}(k) \sum_{\alpha,\beta\in\mathcal{I}_k^+} \Big(\sum_{\gamma\in\mathcal{I}_k^+} |\sinh(K(k))_{\gamma,\alpha}|^2 \Big)^{1/2} \|(\mathcal{N}+1)^{1/2}\Omega\| \|\mathfrak{E}_\beta(k,1)\Omega\|.
\end{aligned}$$

By applying Cauchy–Schwarz in α and in β and by using $|\mathcal{I}_k| = I_k \leq M/2$, we find

$$|\mathfrak{E}_{\mathrm{int}}^{(1,1)}| \leq C\hbar \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \hat{V}(k) \|\sinh(K(k))\|_{\mathrm{HS}} \|(\mathcal{N}+1)^{1/2}\Omega\| \Big(\sum_{\beta\in\mathcal{I}_k^+} \|\mathfrak{E}_\beta(k,1)\Omega\|^2 \Big)^{1/2}.$$

With (5.18) we get

$$|\mathfrak{E}_{\mathrm{int}}^{(1,1)}| \leq \frac{C\hbar}{\mathfrak{n}^2} N^\mu \sup_{\lambda\in[0,1]} \|(\mathcal{N}+2)^{3/2} T_\lambda \Omega\| \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \hat{V}(k) e^{2\|K(k)\|_{\mathrm{HS}}} \sum_{l\in\Gamma^{\mathrm{nor}}} \|K(l)\|_{\mathrm{HS}}.$$

As before, Lemma 5.5 and Proposition 5.6 show that $|\mathfrak{E}_{\mathrm{int}}^{(1,1)}| \leq C\frac{\hbar}{\mathfrak{n}^2} N^{2\mu}$. Analogously, we obtain $|\mathfrak{E}_{\mathrm{int}}^{(1,2)}| \leq C\frac{\hbar}{\mathfrak{n}^2} N^{2\mu}$. We conclude that $|\mathfrak{E}_{\mathrm{int}}^{(1)}| \leq C\frac{\hbar}{\mathfrak{n}^2} N^{3\mu}$ The error term $\mathfrak{E}_{\mathrm{int}}^{(2)}$ differs from $\mathfrak{E}_{\mathrm{int}}^{(1)}$ only in the replacement of the index set $\mathcal{I}_k^+$ by $\mathcal{I}_k^-$. Therefore, we find $|\mathfrak{E}_{\mathrm{int}}^{(2)}| \leq C\frac{\hbar}{\mathfrak{n}^2} N^{3\mu}$. As for the error term $\mathfrak{E}_{\mathrm{int}}^{(3)}$, it also differs from $\mathfrak{E}_{\mathrm{int}}^{(1)}$ in the index set, some hermitian conjugations, and the appearance of a cosh instead of a sinh. The estimates however remain valid and we also obtain $|\mathfrak{E}_{\mathrm{int}}^{(3)}| \leq C\frac{\hbar}{\mathfrak{n}^2} N^{3\mu}$. □

6.5 Proof of Theorem 3.2

Now that we have evaluated the expectation values we are finally able to proof Theorem 3.2. This is the content of this section. We are left with evaluating the traces of the expectation value of the kinetic energy and of the interaction energy. We will show that these traces reproduce the Gell-Mann–Brueckner formula.

Proof of Theorem 3.2. Recall the definition of the correlation Hamiltonian (4.7) and the decomposition (4.8) of the quadratic interaction Q_N. Combining the results of the previous chapter we conclude that

$$\begin{aligned}&\langle \xi, \mathcal{H}_{\mathrm{corr}}\xi\rangle \\ &= \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k| \mathrm{tr}\Big((D(k)+W(k))\sinh^2(K(k)) + \tilde{W}(k)\sinh(K(k))\cosh(K(k))\Big) + \mathfrak{E}\end{aligned}$$

where the error $\mathfrak{E}$ fulfills

$$|\mathfrak{E}| \leq C\Big[\frac{1}{N} + \frac{1}{M} + \frac{\hbar}{\mathfrak{n}^2}N^{3\mu} + \hbar N^{-\delta/2+\mu}\Big]$$

with $\hbar = N^{-1/3}$ and $\mathfrak{n} = N^{1/3-\delta/2}M^{-1/2}$. We want to evaluate the traces. For that, notice that by definition (5.14) of K(k) we have

$$\sinh(K(k)) = \frac{1}{2}\big(|S_1(k)^T| - |S_1(k)^T|^{-1}\big), \quad \cosh(K(k)) = \frac{1}{2}\big(|S_1(k)^T| + |S_1(k)^T|^{-1}\big).$$

Notice that $S_1(k)S_1(k)^T = |S_1(k)^T|^2$ and $\big(|S_1(k)^T|^{-1}\big)^2 = S_2(k)S_2(k)^T$, where

$$S_2(k) = \Big(D(k) + W(k) - \tilde{W}(k)\Big)^{-1/2} E(k)^{1/2}.$$

Consequently

$$\begin{aligned}\sinh(K(k))\cosh(K(k)) &= \frac{1}{4}\big(|S_1(k)^T| - |S_1(k)^T|^{-1}\big)^T\big(|S_1(k)^T| + |S_1(k)^T|^{-1}\big) \\ &= \frac{1}{4}\big(S_1(k)S_1(k)^T - S_2(k)S_2(k)^T\big),\end{aligned}$$

and

$$\begin{aligned}\sinh^2(K(k)) &= \frac{1}{4}\big(|S_1(k)^T| - |S_1(k)^T|^{-1}\big)^T\big(|S_1(k)^T| - |S_1(k)^T|^{-1}\big) \\ &= \frac{1}{4}\big(S_1(k)S_1(k)^T + S_2(k)S_2(k)^T - 2\mathbb{I}\big).\end{aligned}$$

Using the explicit Form (5.16) of $S_1(k)$, $E(k)$, and $S_2(k)$, the expectation value $\langle \xi, \mathcal{H}_{\mathrm{corr}}\xi\rangle$

can be simplified to

$$\begin{aligned}\langle \xi, \mathcal{H}_{\rm corr}\xi\rangle &= \frac{\hbar\kappa}{4}\sum_{k\in\Gamma^{\rm nor}}|k|\Big[\mathrm{tr}\Big(\big(D(k)+W(k)+\tilde W(k)\big)S_1(k)S_1(k)^T\Big)\\ &\quad+\mathrm{tr}\Big(\big(D(k)+W(k)-\tilde W(k)\big)S_2(k)S_2(k)^T\Big)\Big]\\ &\quad-\frac{\hbar\kappa}{2}\sum_{k\in\Gamma^{\rm nor}}|k|\mathrm{tr}\big(D(k)+W(k)\big)+\mathfrak{E}\\ &=\hbar\kappa\sum_{k\in\Gamma^{\rm nor}}|k|\Big(\frac{1}{2}\mathrm{tr}\,E(k)-\frac{1}{2}\mathrm{tr}\big(D(k)+W(k)\big)\Big)+\mathfrak{E}. \end{aligned}\tag{6.15}$$

The next task is to evaluate the traces in (6.15).

Evaluation of the Traces. For simplicity, we shall drop the k-dependence in the notation (we will restore it in (6.18)). Recall the block diagonalization (5.24), by which

$$\begin{aligned}\frac{1}{2}\mathrm{tr}E &= \frac{1}{2}\mathrm{tr}\left[\begin{pmatrix}d & 0\\ 0 & d+2b\end{pmatrix}^{1/2}\begin{pmatrix}d+2b & 0\\ 0 & d\end{pmatrix}\begin{pmatrix}d & 0\\ 0 & d+2b\end{pmatrix}^{1/2}\right]^{1/2}\\ &=\frac{1}{2}\mathrm{tr}\begin{pmatrix}d^{1/2}(d+2b)d^{1/2} & 0\\ 0 & (d+2b)^{1/2}d(d+2b)^{1/2}\end{pmatrix}^{1/2}\\ &=\frac{1}{2}\mathrm{tr}\Big[d^{1/2}(d+2b)d^{1/2}\Big]^{1/2}+\frac{1}{2}\mathrm{tr}\Big[(d+2b)^{1/2}d(d+2b)^{1/2}\Big]^{1/2}\\ &=\mathrm{tr}\Big[d^{1/2}(d+2b)d^{1/2}\Big]^{1/2}, \end{aligned}\tag{6.16}$$

because $d^{1/2}(d+2b)d^{1/2}$ and $(d+2b)^{1/2}d(d+2b)^{1/2}$ have the same spectrum (because $\sigma(AB)=\sigma(BA)$ for positive operators). To calculate this trace, recall that $d=\mathrm{diag}(u_\alpha^2:\alpha=1,\dots,I)$ and $b_{\alpha,\beta}=gv_\alpha v_\beta$. Notice that for a matrix multiplication ABA, where $A=\mathrm{diag}(a_i)$ is a diagonalized matrix and B is of the form $B_{i,j}=b_ib_j$, we have

$$(ABA)_{i,j}=b_ib_ja_ia_j=\Big(|u\rangle\langle u|\Big)_{i,j}\quad\text{with } u=(a_1b_1,\dots,a_nb_n).$$

We conclude that $(d^{1/2}bd^{1/2})_{\alpha,\beta}=gu_\alpha u_bv_\alpha v_\beta$

$$d^{1/2}(d+2b)d^{1/2}=d^2+2g\,|\tilde u\rangle\langle\tilde u|$$

is a rank-one perturbation of a diagonal operator, with diagonal part $d^2=\mathrm{diag}(u_\alpha^4:\alpha=1,\dots,I)$ and with $\tilde u=(v_1u_1,\dots,v_Iu_I)\in\mathbb{R}^I$. Note that for any invertible matrix $A\in\mathbb{C}^{n\times n}$, and for any $x,y\in\mathbb{C}^n$,

$$(A+|x\rangle\langle y|)^{-1}=A^{-1}-\frac{A^{-1}|x\rangle\langle y|A^{-1}}{1+\langle y,A^{-1}x\rangle},$$

whenever the r.h.s. is well-defined. This can be used to calculate the resolvent of a matrix with rank-one perturbation. For any $\lambda\in[0,\infty)$ we find

$$\big(d^2+2g\,|\tilde u\rangle\langle\tilde u|+\lambda^2\big)^{-1}=(d^2+\lambda^2)^{-1}-\frac{2g}{1+2g\sum_{\alpha=1}^I\frac{u_a^2v_a^2}{u_\alpha^4+\lambda^2}}\,|w\rangle\langle w|\tag{6.17}$$

with $w \in \mathbb{R}^I$ defined by $w_\alpha := u_\alpha v_\alpha (u_\alpha^4 + \lambda^2)^{-1}$. We can write $\sqrt{x} = 2/\pi \int_0^\infty \mathbb{I} - \lambda^2/(x + \lambda^2)\mathrm{d}\lambda$. By functional calculus, the square root of a non-negative operator A is

$$\sqrt{A} = \frac{2}{\pi}\int_0^\infty \Big(\mathbb{I} - \frac{\lambda^2}{A+\lambda^2}\Big)\mathrm{d}\lambda.$$

Using the integral identity we find

$$\begin{aligned}\mathrm{tr}\big[d^{1/2}(d+2b)d^{1/2}\big]^{1/2} &= \frac{2}{\pi}\int_0^\infty \mathrm{tr}\Big(\mathbb{I} - \frac{\lambda^2}{d^2+\lambda^2}\Big)\mathrm{d}\lambda + \frac{2}{\pi}\int_0^\infty \frac{\lambda^2 2g}{1+2g\sum_{\alpha=1}^I \frac{u_\alpha^2 v_\alpha^2}{u_\alpha^4+\lambda^2}}\|w\|^2\mathrm{d}\lambda \\ &= \mathrm{tr}\, d + \frac{2}{\pi}\int_0^\infty \frac{\lambda^2}{1+2g\sum_{\alpha=1}^I \frac{u_\alpha^2 v_\alpha^2}{u_\alpha^4+\lambda^2}} 2g \sum_{\alpha=1}^I \frac{u_\alpha^2 v_\alpha^2}{(u_\alpha^4+\lambda^2)^2}\mathrm{d}\lambda\end{aligned}$$

where we used (6.17) and that $\mathrm{tr}\,|w\rangle\langle w| = \|w\|^2$. Restoring the k-dependence and let

$$f_k(\lambda) := 1 + 2g(k)\sum_{\alpha=1}^{I_k} \frac{u_\alpha(k)^2 v_\alpha(k)^2}{u_\alpha(k)^4+\lambda^2}.$$

It holds that

$$f_k'(\lambda) = -2g(k)\sum_{\alpha=1}^{I_k} \frac{2\lambda u_\alpha(k)^2 v_\alpha(k)^2}{(u_\alpha(k)^4+\lambda^2)^2}.$$

With integration by parts (noting that the boundary terms vanishes since $\log f_k(\lambda) \sim 1/\lambda^2$) and with $\mathrm{tr}\, d = 1/2\mathrm{tr}\, D$ we get

$$\mathrm{tr}\big[d^{1/2}(d+2b)d^{1/2}\big]^{1/2} = \frac{1}{2}\mathrm{tr}\, D - \frac{1}{\pi}\int_0^\infty \lambda \frac{f_k'(\lambda)}{f_k(\lambda)}\mathrm{d}\lambda = \frac{1}{2}\mathrm{tr}\, D + \frac{1}{\pi}\int_0^\infty \log f_k(\lambda)\mathrm{d}\lambda.$$

Inserting this expression in (6.16) and then in (6.15), we obtain

$$\langle \xi, \mathcal{H}_{\mathrm{corr}}\xi\rangle = \hbar\kappa \sum_{k\in\Gamma^{\mathrm{nor}}} |k|\Big(\frac{1}{\pi}\int_0^\infty \log f_k(\lambda)\mathrm{d}\lambda - g(k)\sum_{\alpha=1}^{I_k} v_\alpha(k)^2\Big) + \mathfrak{E} \tag{6.18}$$

where we used that, according to (5.23), $\mathrm{tr}\, W = 2\mathrm{tr}\, b = 2g\sum_{\alpha=1}^{I_k} v_\alpha(k)^2$.

Convergence to the Gell-Mann–Brueckner formula. To conclude the proof of Theorem 3.2, we show that (6.18) reproduces the Gell-Mann–Brueckner formula as stated in the theorem. Let

$$\tilde{f}_k(\lambda) := 1 + 4\pi g(k)\Big(1 - \lambda \arctan\Big(\frac{1}{\lambda}\Big)\Big).$$

We claim that

$$\begin{aligned}&\Big|\Big(\frac{1}{\pi}\int_0^\infty \log f_k(\lambda)\mathrm{d}\lambda - g(k)\sum_{\alpha=1}^{I_k} v_\alpha(k)^2\Big) - \Big(\frac{1}{\pi}\int_0^\infty \log \tilde{f}_k(\lambda)\mathrm{d}\lambda - g(k)\pi\Big)\Big| \\ &\le C\Big(M^{1/4}N^{-\frac{1}{6}+\frac{\delta}{2}+\frac{\mu}{2}} + N^{-\delta/2} + M^{-1/4}N^{\delta/2}\Big).\end{aligned} \tag{6.19}$$

Since $\log \tilde{f}_k(\lambda) = g(k) = 0$ for all $|k| > N^\mu$, inserting (6.19) into (6.18) we obtain

$$\langle \xi, \mathcal{H}_{\mathrm{corr}} \xi \rangle = \hbar\kappa \sum_{k \in \Gamma^{\mathrm{nor}}} |k| \Big(\frac{1}{\pi} \int_0^\infty \log \Big[1 + 4\pi g(k) \Big(1 - \lambda \arctan\Big(\frac{1}{\lambda} \Big) \Big) \Big] \mathrm{d}\lambda - g(k)\pi \Big) + \tilde{\mathfrak{E}}$$

with an error

$$|\tilde{\mathfrak{E}}| \leq C \Big[N^{-1} + M^{-1} + \frac{\hbar N^{3\mu}}{\mathfrak{n}^2} + \hbar N^{-\delta/2+\mu} \Big] + C\hbar \Big[M^{1/4} N^{-1/6+\delta/2+\mu/2} + N^{-\delta/2} + M^{-1/4} N^{\delta/2} \Big]. \tag{6.20}$$

Replacing the sum over $k \in \Gamma^{\mathrm{nor}}$ by $1/2$ times the sum over $k \in \mathbb{Z}^3$, and replacing $\kappa = \kappa_0 + \mathcal{O}(N^{-1/3})$ by $\kappa_0 = (3/4\pi)^{1/3}$ (using also the Lipschitz continuity of the logarithm), we arrive at (3.2).

We still have to show (6.19). For this, recall from Proposition 4.1 that, in terms of the surface measure σ of the patch p_α on the unit sphere, we have

$$v_\alpha(k)^2 = \sigma(p_\alpha) u_\alpha(k)^2 \Big(1 + \mathcal{O}\Big(\sqrt{M} N^{-1/3+\delta+\mu} \Big) \Big).$$

Thus

$$\begin{aligned} f_k(\lambda) &= 1 + 2g(k) \sum_{\alpha=1}^{I_k} \frac{u_\alpha(k)^2 v_\alpha(k)^2}{u_\alpha(k)^4 + \lambda} \\ &= 1 + 2g(k) \sum_{\alpha=1}^{I_k} \sigma(p_\alpha) \frac{u_\alpha(k)^4}{u_\alpha(k)^4 + \lambda^2} + \mathcal{O}\Big(\sqrt{M} N^{-1/3+\delta+\mu} \Big). \end{aligned}$$

The Riemann sum is approximated by the corresponding surface integral over a subset of $\mathbb{S}^2$. We write $\cos\theta_\alpha = \hat{k} \cdot \hat{\omega}_\alpha = u_\alpha(k)^2$ and ϕ_α for the azimuth of ω_α. We parametrize the surface integral in the same spherical coordinate system. (The inclination θ is measured with respect to k, and the azimuth ϕ in the plane perpendicular to k.) We estimate every summand by

$$\begin{aligned} &\Big| \int_{p_\alpha} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma - \sigma(p_\alpha) \frac{\cos^2\theta_\alpha}{\cos^2\theta_\alpha + \lambda^2} \Big| \\ &\leq \int_{p_\alpha} \Big| \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} - \frac{\cos^2\theta_\alpha}{\cos^2\theta_\alpha + \lambda^2} \Big| \mathrm{d}\sigma \\ &\leq \iint_{\hat{\omega}(\theta,\phi) \in p_\alpha} \Big| \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} - \frac{\cos^2\theta_\alpha}{\cos^2\theta_\alpha + \lambda^2} \Big| |\sin\theta| \mathrm{d}\theta \mathrm{d}\phi. \end{aligned}$$

By the supremum of the derivative and the bound of the diameter, $\sup_{(\theta,\phi)\in p_\alpha} |\theta - \theta_\alpha| \leq C/\sqrt{M}$ we find that

$$\Big| \int_{p_\alpha} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma - \sigma(p_\alpha) \frac{\cos^2\theta_\alpha}{\cos^2\theta_\alpha + \lambda^2} \Big| \leq \sup_{\hat{\omega}(\theta,\phi)\in p_\alpha} \Big| \frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \Big| \frac{C}{\sqrt{M}} \sigma(p_\alpha). \tag{6.21}$$

The derivative is bounded by

$$\Big| \frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \Big| = 2 \frac{\lambda^2}{\cos^2\theta + \lambda^2} \frac{|\cos\theta||\sin\theta|}{\cos^2\theta + \lambda^2} \leq \frac{2}{|\cos\theta|}$$

where we used that the first factor is bounded by 1 and the second by $1/|\cos\theta|$. Recall that $\alpha \in \{1, 2, \dots, I_k\}$, which by definition of the index implies $\cos\theta_\alpha > N^{-\delta}$. The bound $|\theta - \theta_\alpha| \leq CM^{-1/2}$ implies that also $\cos\theta > CN^{-\delta}$. So (6.21) implies

$$\Big| \int_{p_\alpha} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma - \sigma(p_\alpha) \frac{\cos^2\theta_\alpha}{\cos^2\theta_\alpha + \lambda^2} \Big| \leq C \frac{N^\delta}{M^{3/2}}.$$

Let $\mathbb{S}^2_{\text{reduced}}$ be the unit half-sphere excluding the collar of width $N^{-\delta}$ and excluding the corridor p_{corri} and note that the number of patches is at most M. We conclude that

$$\Big| \sum_{\alpha=1}^{I_k} \sigma(p_\alpha) \frac{u_\alpha(k)^4}{u_\alpha(k)^4 + \lambda^2} - \int_{\mathbb{S}^2_{\text{reduced}}} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma \Big| \leq C \frac{N^\delta}{\sqrt{M}}.$$

Since $\cos^2\theta/(\cos^2\theta + \lambda^2) \leq 1$ we can compare to the integral over the whole unit half-sphere $\mathbb{S}^2_{\text{half}}$,

$$\Big| \int_{\mathbb{S}^2_{\text{reduced}}} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma - \int_{\mathbb{S}^2_{\text{half}}} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma \Big| \leq C \Big[N^{-\delta} + M^{1/2} N^{-1/3+\mu} \Big].$$

The surface integral over the unit half-sphere can be computed as

$$\int_{\mathbb{S}^2_{\text{half}}} \frac{\cos^2\theta}{\cos^2\theta + \lambda^2} \mathrm{d}\sigma = \int_0^{\pi/2} \sin(\theta) \frac{\cos^2(\theta)}{\cos^2(\theta) + \lambda^2} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi = 2\pi \Big(1 - \lambda \arctan\Big(\frac{1}{\lambda}\Big) \Big). \tag{6.22}$$

Since $g(k) = \kappa \hat{V}(k)$ is uniformly bounded (by assumption on $\hat{V}$), we conclude that

$$\big| f(\lambda) - \tilde{f}(\lambda) \big| \leq C \Big(\sqrt{M} N^{-\frac{1}{3}+\delta+\mu} + N^{-\delta} + \frac{N^\delta}{\sqrt{M}} \Big).$$

For $x \geq 0$ the function $x \mapsto \log(1+x)$ has Lipschitz constant 1. Therefore, we get

$$\big| \log f(\lambda) - \log \tilde{f}(\lambda) \big| \leq C \Big(\sqrt{M} N^{-\frac{1}{3}+\delta+\mu} + N^{-\delta} + \frac{N^\delta}{\sqrt{M}} \Big).$$

It remains to compare the integrals over λ. For this task, we will split the integral at some $\Lambda > 0$. For the integral over $[0, \Lambda]$ we can use this bound. However, for the integral from Λ to infinity, we need to find another bound.

Since $\log(1+x) \leq x$ for all $x \geq 0$, we have

$$|\log f(\lambda)| \leq 2g(k) \sum_{\alpha=1}^{I_k} \sigma(p_\alpha) \frac{u_\alpha(k)^4}{u_\alpha(k)^4 + \lambda^2} \leq 2g(k) \sum_{\alpha=1}^{I_k} \frac{C}{M} \frac{1}{\lambda^2} \leq \frac{C}{\lambda^2},$$

where we used the two inequalities $0 \leq u_\alpha(k)^4 \leq 1$. Using the integral Identity (6.22) (it follows from the l.h.s. that we can bound the expression form above by $1/\lambda^2 \int \cos^2\theta \mathrm{d}\sigma$) we can see that

$$\big| \log \tilde{f}(\lambda) \big| \leq 4\pi g(k) \big| 1 - \lambda \arctan\Big(\frac{1}{\lambda}\Big) \big| \leq \frac{C}{\lambda^2}$$

Now we are ready to split the integral at some $\Lambda > 0$. Using the last three estimates and optimizing over Λ yields

$$\begin{aligned}
&\Big|\frac{1}{\pi}\int_0^\infty \log f(\lambda)\mathrm{d}\lambda - \frac{1}{\pi}\int_0^\infty \log \tilde{f}(\lambda)\mathrm{d}\lambda\Big| \\
&\leq \frac{1}{\pi}\int_0^\Lambda \Big|\log f(\lambda) - \log\tilde{f}(\lambda)\Big|\mathrm{d}\lambda + \frac{1}{\pi}\int_\Lambda^\infty \frac{C}{\lambda^2}\mathrm{d}\lambda \\
&\leq C\Lambda\Big(\sqrt{M}N^{-\frac{1}{3}+\delta+\mu} + N^{-\delta} + \frac{N^\delta}{\sqrt{M}}\Big) + C\Lambda^{-1} \\
&\leq C\Big(M^{1/4}N^{-\frac{1}{6}+\frac{\delta}{2}+\frac{\mu}{2}} + N^{-\frac{\delta}{2}} + M^{-\frac{1}{4}}N^{\frac{\delta}{2}}\Big). \qquad (6.23)
\end{aligned}$$

For the last estimate we used the fact that for any $a \in \mathbb{R}_{>0}$ the minimum of $ax + 1/x$ is attained at $x = 1/\sqrt{a}$. By a similar Riemann sum argument we obtain

$$-g(k)\sum_{\alpha=1}^{I_k} v_\alpha^2(k) = -g(k)\pi + \mathcal{O}\Big(\sqrt{M}N^{-\frac{1}{3}+\delta+\mu} + N^{-\delta}\Big).$$

Indeed, we have

$$-g(k)\sum_{\alpha=1}^{I_k} v_\alpha(k)^2 = -g(k)\sum_{\alpha=1}^{I_k}\sigma(p_\alpha)u_\alpha(k)^2 + \mathcal{O}\Big(\sqrt{M}N^{-\frac{1}{3}+\delta+\mu}\Big).$$

Similar arguments yields

$$\begin{aligned}
\Big|\int_{p_\alpha}\cos\theta\mathrm{d}\sigma - \sigma(p_\alpha)\cos\theta_\alpha\Big| &\leq \int_{p_\alpha}|\cos\theta - \cos\theta_\alpha|\mathrm{d}\sigma \\
&\leq \iint_{\hat{\omega}(\theta,\phi)\in p_\alpha}|\cos\theta - \cos\theta_\alpha||\sin\theta|\mathrm{d}\theta\mathrm{d}\phi \\
&\leq \sup_{\hat{\omega}(\theta,\phi)\in p_\alpha}\Big|\frac{\mathrm{d}}{\mathrm{d}\theta}\cos\theta\Big|\frac{C}{\sqrt{M}}\sigma(p_\alpha) \leq \frac{C}{M^{3/2}}.
\end{aligned}$$

We conclude that

$$\Big|\sum_{\alpha=1}^{I_k}\sigma(p_\alpha)u_\alpha(k)^2 - \int_{\mathbb{S}^2_{\text{reduced}}}\cos\theta\mathrm{d}\sigma\Big| \leq \frac{C}{\sqrt{M}}.$$

We can compare the integral over the whole unit half-sphere, using $\cos\theta \leq 1$,

$$\Big|\int_{\mathbb{S}^2_{\text{reduced}}}\cos\theta\mathrm{d}\sigma - \int_{\mathbb{S}^2_{\text{half}}}\cos\theta\mathrm{d}\sigma\Big| \leq C\Big[N^{-\delta} + M^{1/2}N^{-1/3+\mu}\Big]$$

From $\int_{\mathbb{S}^2_{\text{half}}}\cos\theta\mathrm{d}\sigma = \pi$ and form the fact that $g(k)$ is uniformly bounded it follows that

$$\begin{aligned}
\Big|g(k)\sum_{\alpha=1}^{I_k} v_\alpha(k)^2 - g(k)\pi\Big| &\leq C\Big[N^{-\delta} + \frac{1}{\sqrt{M}} + \sqrt{M}N^{-\frac{1}{3}+\delta+\mu}\Big] \\
&\leq C\Big[N^{-\delta} + \sqrt{M}N^{-\frac{1}{3}+\delta+\mu}\Big].
\end{aligned}$$

where the error is smaller than (6.23) (we assumed that $-1/6 + \epsilon/2 + \delta + \mu < 0$). This completes the proof of (6.19). □

Chapter 7

Proof of the Main Theorem

In the previous chapters, we proved that the correlation energy can be determined up to an error by the Gell-Mann–Brueckner formula for a N-particle system with suitable conditions on the potential V. In this chapter we present the proof of Theorem 3.1 by the help of Theorem 3.2.

7.1 Proof of Theorem 3.1

As already mentioned, in the last few chapters we proved a slightly different version of Theorem 3.1, assuming that the potential $\hat{V}$ has compact support and that the radius of the support depends on N. For weaker condition on the potential, we will cut off the potential at N^μ and we will use the statement about compact supported potentials. Then we will prove that the contribution of the cut off part is sufficiently small.

Proof of Theorem 3.1. Recall that

$$H_N = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{x_i} + \frac{1}{N}\sum_{1\le i<j\le N} V(x_i - x_j)$$

is the Hamiltonian with a potential V such that $\hat{V}$ is non-negative and $\int \hat{V}(p)|p|^n \mathrm{d}p < \infty$ for an $n > 24$. We cut off $\hat{V}$ at N^μ, with $0 < \mu < 1/6$ chosen later, and we define

$$V_n := \mathcal{F}^{-1}\Big(\hat{V}(p)\chi(|p| < N^\mu)\Big) \qquad \text{and}$$

$$\tilde{H}_N := -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{x_i} + \frac{1}{N}\sum_{1\le i<j\le N} V_N(x_i - x_j).$$

Then the expectation value in a state $\psi \in L^2_a(\mathbb{T}^{3N})$ can be split in

$$\langle \psi, H_N\psi\rangle = \langle \psi, \tilde{H}_N\psi\rangle + \frac{1}{N}\sum_{1\le i<j\le N}\langle \psi, (V - V_N)\psi\rangle. \tag{7.1}$$

The expectation value of $(V - V_N)$ can be controlled by using

$$\begin{aligned}
&\Big|\langle\psi, \Big(V(x_1 - x_2) - V_N(x_1 - x_2)\Big)\psi\rangle\Big| \leq \Big|\sum_{p\in\mathbb{Z}^3}\Big(\hat{V}(p) - \hat{V}_N(p)\Big)\langle\psi, e^{ip(x_1-x_2)}\psi\rangle\Big| \\
&\leq \sum_{p\in\mathbb{Z}^3}\Big|\hat{V}(p) - \hat{V}(p)\chi(|p| < N^\mu)\Big| = \sum_{p\in\mathbb{Z}^3}\hat{V}(p)\chi(|p| \geq N^\mu) \\
&\leq \sum_{p\in\mathbb{Z}^3}\frac{|p|^n}{N^{\mu n}}|\hat{V}(p)| \leq \frac{1}{N^{\mu n}}\sum_{p\in\mathbb{Z}^3}|p|^n\hat{V}(p). \qquad (7.2)
\end{aligned}$$

We used that $\chi(|p| \geq N^\mu) = \chi(\frac{|p|}{N^\mu} \geq 1) \leq (\frac{|p|}{N^\mu})^n$. (This inequality is true for any non-negative number n.) With (7.2) and the assumption $\sum_{p\in\mathbb{Z}^3}|p|^n\hat{V}(p)\mathrm{d}p < \infty$ we find

$$\frac{1}{N}\sum_{1\leq i<j\leq N}\langle\psi, (V - V_N)\psi\rangle = \mathcal{O}\Big(N^{1-\mu n}\Big) = \hbar\mathcal{O}\Big(N^{4/3-\mu n}\Big). \qquad (7.3)$$

The ground state energy, $\tilde{E}_N$, of $\tilde{H}_N$ can be bounded from above by Theorem 3.2, namely for $0 < \varepsilon < 1/3 - 2\mu$ and $0 < \delta < 1/6 - \varepsilon/2 - \mu$ chosen later, we have

$$\begin{aligned}
\tilde{E}_N &\leq \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}}) \\
&\quad + \frac{\hbar\kappa_0}{2m}\sum_{\substack{|k|\in\mathbb{Z}^3,\\ |k|<N^\mu}}|k|\left[\frac{1}{\pi}\int_0^\infty \log\left(1 + 4\pi\hat{V}(k)m\kappa_0\Big(1 - \lambda\arctan\frac{1}{\lambda}\Big)\right)\mathrm{d}\lambda - \hat{V}(k)m\kappa_0\pi\right] \\
&\quad + \hbar\mathcal{O}\Big(N^{-\epsilon} + MN^{-2/3+\delta+3\mu} + N^{-\delta/2+\mu} + M^{1/4}N^{-1/6+\delta/2+\mu/2}\Big) \qquad (7.4)
\end{aligned}$$

with $M = N^{1/3+\varepsilon}$. By (7.1), (7.3) and (7.4) we conclude that

$$\begin{aligned}
E_N &\leq \tilde{E}_N + C\hbar\Big(N^{4/3-\mu n}\Big) \\
&\leq \mathcal{E}_{\mathrm{HF}}(\omega_{\mathrm{pw}}) \\
&\quad + \frac{\hbar\kappa_0}{2m}\sum_{\substack{|k|\in\mathbb{Z}^3,\\ |k|<N^\mu}}|k|\left[\frac{1}{\pi}\int_0^\infty \log\left(1 + 4\pi\hat{V}(k)m\kappa_0\Big(1 - \lambda\arctan\frac{1}{\lambda}\Big)\right)\mathrm{d}\lambda - \hat{V}(k)m\kappa_0\pi\right] \\
&\quad + \hbar\mathcal{O}\Big(N^{-\epsilon} + MN^{-2/3+\delta+3\mu} + N^{-\delta/2+\mu} + M^{1/4}N^{-1/6+\delta/2+\mu/2} + N^{4/3-\mu n}\Big).
\end{aligned}$$

The error term is optimized with the choices

$$\epsilon = \frac{n-24}{27n+18}, \qquad \mu = \frac{37}{27n+18}, \qquad \delta = \frac{2n+26}{27n+18}.$$

These choices imply that the error term is of order $\hbar N^{-\frac{n-24}{27n+18}}$. To complete the proof we need to show that

$$\frac{\hbar\kappa_0}{2m}\sum_{\substack{k\in\mathbb{Z}^3,\\ |k|\geq N^\mu}}|k|\left[\frac{1}{\pi}\int_0^\infty \log\left(1 + 4\pi\hat{V}(k)m\kappa_0\Big(1 - \lambda\arctan\frac{1}{\lambda}\Big)\right)\mathrm{d}\lambda - \hat{V}(k)m\kappa_0\pi\right] \qquad (7.5)$$

is equal to $o(\hbar)$. First, for fixed k we consider the expression

$$\frac{1}{\pi}\int_0^\infty \log\left(1+4\hat{V}(k)m\kappa_0\Big(1-\lambda\arctan\frac{1}{\lambda}\Big)\right)\mathrm{d}\lambda.$$

Using the Taylor expansion of the logarithm $\log(1+x)=\sum_{j=1}^\infty(-1)^{j+1}x^j/j\leq x+Cx^2$ for $|x|<1$ we find

$$\begin{aligned}\leq&\frac{1}{\pi}\int_0^\infty 4\pi\hat{V}(k)m\kappa_0\Big(1-\lambda\arctan\frac{1}{\lambda}\Big)\mathrm{d}\lambda+C\frac{1}{\pi}\int_0^\infty\left(4\pi\hat{V}(k)m\kappa_0\Big(1-\lambda\arctan\frac{1}{\lambda}\Big)\right)^2\mathrm{d}\lambda\\ =&\hat{V}(k)m\kappa_0\pi+C\frac{1}{\pi}\int_0^\infty\left(4\pi\hat{V}(k)m\kappa_0\Big(1-\lambda\arctan\frac{1}{\lambda}\Big)\right)^2\mathrm{d}\lambda=\hat{V}(k)m\kappa_0\pi+C\hat{V}(k)^2.\end{aligned}$$

Inserting this term into (7.5) we get that this term is equal to

$$C\hbar\sum_{\substack{k\in\mathbb{Z}^3,\\ |k|\geq N^\mu}}|k|\hat{V}(k)^2\leq C\hbar\sum_{\substack{k\in\mathbb{Z}^3,\\ |k|\geq N^\mu}}\Big(|k|\hat{V}(k)\Big)^2\leq C\hbar\Big[\sum_{\substack{k\in\mathbb{Z}^3,\\ |k|\geq N^\mu}}|k|\hat{V}(k)\Big]^2=o(\hbar)$$

where we used that $\hat{V}$ is a non-negative function and that $\sum_{p\in\mathbb{Z}^3}|p|^n\hat{V}(p)<\infty$. This completes the proof of the main theorem. □

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