The Ground State Energy of a Dilute Bose Gas in Dimension $n \geq 3$

PhD Dissertation

by Anders Aaen

January 14, 2014

Advisor: Søren Fournais
Department of Mathematics
Aarhus University

Contents

Preface

The theory of quantum mechanics provides a mathematical model for describing interacting systems of microscopic particles. However, to do actual calculations with the model can be a complicated matter, and many basic properties remain to be understood. A particular fundamental problem is the ground state energy of the interacting Bose gas. Even this problem is, in its full generality, beyond reach of a mathematical treatment. If one considers a sufficiently dilute Bose gas, it is possible to do something though. Using semi-rigorous methods, asymptotic low density formulas for the ground state energy was derived by Bogoliubov in the 1940's and by Lee, Huang and Yang in the 1950's. Subsequently many attempts were made to extract rigorous results from their methods, but only with modest success. For a rather long period of time the subject was quiescent. Now, starting with the experimental realization of Bose-Einstein condensation in 1995, modern technology has shown it possible to test theoretical predictions for Bose gasses in labs, which in turns has inspired a renewed interest in a rigorous understanding of these important physical systems.

The present dissertation is the result of my Ph.D.-studies at the Department of Mathematics, Aarhus University. The aim of the project was to investigate the ground state energy of a Bose gas in 4 spatial dimensions, motivated by a recent, but non-rigorous, calculation of Yang. I have succeeded to obtain rigorous results verifying Yang's prediction to some precision (the leading order term), and almost consistent to higher precision (the correction term). It turned out that some of the rigorous 3-dimensional methods may rather easily be applied in higher dimensions, while others cannot (at all?). I concluded the latter after having considered a somewhat new approach, introduced by Yau and Yin, in 4 dimensions. Instead I was able to make a substantial simplification of their approach, and hence the title of my dissertation contains also dimension $n = 3$.

There are several people I wish to thank. First and foremost I would like to thank my advisor Professor Søren Fournais for his major commitment and patient guiding. I would also like to thank Professor Jan Philip Solovej for helpful discussions on the topic in chapter 4. Part of the project was carried out while I was traveling around the world, profiting from the Danish fellowship 'Rejselegat for Matematikere'. In this regard, I would like to thank Professor Rod Gover at the Department of Mathematics, University of Auckland, and Professor Thomas Østergaard Sørensen at the Department of Mathematics, Ludwig Maximillians University, München. I would like to thank Matthias Engelmann for proof-reading part of the manuscript. Finally, I thank my wife, Louisa, and our three children Marius, Elise and Bertram for your love and support.

Abstract

We consider a Bose gas in spatial dimension $n \geq 3$ with a repulsive, radially symmetric two-body potential V. In the limit of low density ρ, the ground state energy per particle in the thermodynamic limit is shown to be $(n-2)|\mathbb{S}^{n-1}|a^{n-2}\rho$, where $|\mathbb{S}^{n-1}|$ denotes the surface measure of the unit sphere in $\mathbb{R}^n$, and a is the scattering length of V. Furthermore, for smooth and compactly supported two-body potentials, we derive an upper bound to the ground state energy with a correction term $(1+\gamma)8\pi^4a^6\rho^2|\ln(a^4\rho)|$ in 4 dimensions, where $0 < \gamma \leq C\|V\|_\infty^{1/2}\|V\|_1^{1/2}$, and a correction term which is $\mathcal{O}(\rho^2)$ in higher dimensions. Finally, we use a grand canonical construction to give a simplified proof of the second order upper bound to the Lee-Huang-Yang formula, a result first obtained by Yau and Yin. We also test this method in 4 dimensions, but with a negative outcome.

Resume (Danish Abstract)

Vi betragter en Bose gas i rummelig dimension $n \geq 3$ med et positivt, radialt symmetrisk par-potential V. I grænsen af lav tæthed ρ vises det, at grundtilstandsenergien per partikel i den termodynamiske grænse er $(n-2)|\mathbb{S}^{n-1}|a^{n-2}\rho$, hvor $|\mathbb{S}^{n-1}|$ betegner overflademålet af enhedssfæren i $\mathbb{R}^n$, og hvor a er spredningslængden af V. Endvidere, for glatte par-potentialer med kompakt støtte udleder vi en øvre grænse til grundtilstandsenergien med et korrektionsled $(1+\gamma)8\pi^4a^6\rho^2|\ln(a^4\rho)|$ i 4 dimensioner, hvor $0 < \gamma \leq C\|V\|_\infty^{1/2}\|V\|_1^{1/2}$, og med et korrektionsled $\mathcal{O}(\rho^2)$ i højere dimensioner. Endelig anvender vi en grand-kanonisk konstruktion til at give et simplificeret bevis for den øvre grænse til Lee-Huang-Yang formlen, et resultat først opnået af Yau og Yin. Vi afprøver også metoden i 4 dimensioner, men med et negativt udfald.

Chapter 1

Introduction

In this chapter we introduce the model in consideration along with relevant basic concepts. We then discuss previous works by other people, and finally we give an outline of our main results.

1.1 The Interacting Bose Gas

Consider the system of N identical particles in an n-dimensional cubic box $\Lambda = \Lambda_L = (-L/2, L/2)^n$ of side length L. The starting point for a quantum mechanical description of this system is the N-fold tensor product

$$\mathcal{H}_N := \mathcal{H} \otimes \cdots \otimes \mathcal{H} \cong L^2(\Lambda^N) \tag{1.1.1}$$

of the single particle Hilbert space $\mathcal{H} = L^2(\Lambda)$. We assume that the particles are bosons, meaning that we further restrict attention to the symmetric Hilbert space

$$\mathcal{H}_N^{\mathrm{sym}} \cong L^2_{\mathrm{sym}}(\Lambda^N),$$

consisting of all $\Psi \in \mathcal{H}_N$ which are invariant under arbitrary permutations of the N coordinates. The possible states of the system are represented by the unit vectors in $\mathcal{H}_N^{\mathrm{sym}}$, and each physical observable in a state Ψ is given by the expectation value

$$\langle A \rangle_\Psi := \langle \Psi, A\Psi \rangle$$

of a self-adjoint operator A on $\mathcal{H}_N^{\mathrm{sym}}$. The operator corresponding to the total energy of the system is the Hamiltonian

$$H_{N,L} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\Delta_i + U(x_1, \ldots, x_N). \tag{1.1.2}$$

Here $\hbar$ is the reduced Planck constant, m is the mass of a single particle and Δ_i denotes the Laplacian w.r.t. $x_i \in \mathbb{R}^n$. For simplicity we choose units so that $\hbar^2/(2m) = 1$. The sum in (1.1.2) models the total (non-relativistic) kinetic energy of the system, while multiplication with U represents the interactions of the particles. We will assume a *pair-wise* interaction, meaning that U has the form

$$U(x_1, \dots, x_N) = \sum_{1 \le j < k \le N} V(x_j - x_k),$$

for some function V on $\mathbb{R}^n$, usually called the *two-body* potential. Thus our Hamiltonian takes the form

$$H_{N,L} = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le j < k \le N} V(x_j - x_k). \tag{1.1.3}$$

We always assume that V is nonnegative, radially symmetric and Borel measurable. To define $H_{N,L}$ more precisely, we consider the quadratic form

$$Q_{N,L}(\Psi) = \int_{\Lambda^N} \left(\sum_{i=1}^{N} |\nabla_i \Psi|^2 + \sum_{1 \le j < k \le N} V(x_j - x_k)|\Psi|^2 \right) dx_1 \dots dx_N$$

on $L^2_{\mathrm{sym}}(\Lambda^N)$ with appropriate boundary conditions. Usually these are either Dirichlet, periodic or Neumann. That is, we consider $Q_{N,L}$ on either of the domains

$$\mathrm{dom}\big(Q_{N,L}\big) = L^2_{\mathrm{sym}}(\Lambda^N) \cap \begin{cases} H^1(\Lambda^N) & \text{(Neumann)} \\ H^1_{\mathrm{per}}(\Lambda^N) & \text{(periodic)} \\ H^1_0(\Lambda^N) & \text{(Dirichlet)} \end{cases},$$

where $H^1_{\mathrm{per}}(\Lambda^N)$ denotes the set of L-periodic functions in $H^1(\Lambda^N)$, and $H^1_0(\Lambda^N)$ denotes the set of functions in $H^1(\Lambda^N)$ vanishing at the boundary of Λ^N. In either case $Q_{N,L}$ is a closed quadratic form, and it is a well-known fact that the corresponding linear map, which we denote by $H_{N,L}$, is then a self-adjoint operator. The *ground state energy* of the Bose gas is the number

$$E_0(N, L) := \inf\{\langle H_{N,L}\rangle_\Psi : \|\Psi\| = 1\},$$

or equivalently, $E_0(N, L)$ is the lowest eigenvalue of $H_{N,L}$. We are interested in the *thermodynamic limit*, meaning that we let $N, L \to \infty$ in a sequence with fixed density $N/L^n = \rho$. Thus, the ground state energy per particle in the thermodynamic limit is the quantity

$$e_0(\rho) := \lim_{N\to\infty} \frac{E_0(N, (N/\rho)^{1/n})}{N},$$

defined for $\rho > 0$. This limit is well-understood, see e.g. [19]. In particular we will employ the facts that $e_0(\rho)$ is a convex function of ρ and independent of boundary conditions. To calculate $e_0(\rho)$ is one of the most fundamental problems in many-body quantum mechanics. Nevertheless, in its full generality, the problem is at the present stage beyond reach! As we shall see below, there has been significant progress though in understanding the asymptotics of $e_0(\rho)$ in the dilute limit $\rho \to 0$. In this limit the ground state energy depends to some precision only on V via the solution to the two-body problem.

1.2 The Two-Body Problem

In dimension $n \geq 3$ we let
$$s_n := (n-2)|\mathbb{S}^{n-1}|,$$
where $|\mathbb{S}^{n-1}|$ denotes the surface measure of the unit sphere in $\mathbb{R}^n$. Then in particular $s_3 = 4\pi$ and $s_4 = 4\pi^2$.

Definition 1.2.1. Let $n \geq 3$ and suppose that V is a nonnegative, radially symmetric and measurable function on $\mathbb{R}^n$. The *scattering length* of V is the number $a \geq 0$ given by
$$s_n a^{n-2} = \inf_u \int_{\mathbb{R}^n} |\nabla u|^2 + \frac{1}{2} V u^2, \tag{1.2.1}$$
where the infimum is taken over all nonnegative, radially symmetric functions $u \in H^1_{\mathrm{loc}}(\mathbb{R}^n)$ satisfying $u(r) \to 1$ as $r \to \infty$. If the infimum is attained, we call the minimizer a *scattering solution*.

The scattering length in dimension $n = 1, 2$ can be defined using a local version of (1.2.1), see [11]. With the above definition, the scattering length has indeed dimension of length, and hence
$$Y := a^n \rho$$
is a dimensionless quantity. Notice also that a is finite if and only if V is integrable at infinity. Definition 1.2.1 above is motivated by the two-body problem in the limit $L \to \infty$. In fact, it is fairly easy to show the convergence
$$\lim_{L\to\infty} L^n E_0(2, L) = s_n a^{n-2}. \tag{1.2.2}$$
From (1.2.2) we can give a simple heuristic argument for the ground state energy of the general problem. Since we are assuming particles to interact in pairs, we might suggest that the ground state energy of the N-body problem should be close to the ground state energy of the two-body problem times the number of pairs. That is,
$$E_0(N, L) \approx \frac{N(N-1)}{2} E_0(2, L). \tag{1.2.3}$$
Taking the thermodynamic limit and employing (1.2.2), we then obtain
$$e_0(\rho) \approx s_n a^{n-2} \rho. \tag{1.2.4}$$
In fact, (1.2.4) turns out to be true, and we will prove it with rigorous upper and lower bounds. We cannot help remark though, that in light of the complexity of the rigorous proof of (1.2.4), it may seem surprising that the above very simple heuristic argument yields the correct answer! It should also be noted that the approximation (1.2.3) does not apply in dimension $n = 2$ (see e.g. [15]).

The general strategy for an upper bound to $e_0(\rho)$ is to construct a (trial) state with low energy, and which is simple enough to do calculations with. Again, since we are considering a pair-wise interaction of the particles, we might suggest that a good trial state to the general problem can be constructed from the scattering solution. Existence, uniqueness and other properties of the latter are established in the following theorem, which we prove in Appendix 1.A.

Theorem 1.2.2. *Let $n \geq 3$. If $V \in L^1(\mathbb{R}^n)$ is nonnegative, radially symmetric and compactly supported, then the infimum in* (1.2.1) *is a unique minimum, and the minimizer u satisfies the zero-energy scattering equation*

$$-\Delta u + \frac{1}{2} V u = 0 \tag{1.2.5}$$

in the sense of distributions on $\mathbb{R}^n$. Moreover, u is continuous, radially symmetric, radially increasing and satisfies

$$u(r) \geq 1 - (a/r)^{n-2},$$

with equality for $r \geq R_0$, if supp$(V) \subset B(0, R_0)$.

We will consider two alternative representations for the scattering length. Suppose that V satisfies the assumptions of Theorem 1.2.2. Let $1 - w$ denote the corresponding scattering solution, and let

$$\varphi := V w \quad \text{and} \quad g = V - \varphi = V(1 - w).$$

Then w can be represented as

$$w(x) = \frac{1}{2} \Gamma(g)(x) := \frac{1}{2 s_n} \int_{\mathbb{R}^n} \frac{g(y)}{|x - y|^{n-2}} \, dy. \tag{1.2.6}$$

Indeed, $(w - \Gamma(g)/2)$ is a bounded, harmonic function on $\mathbb{R}^n$ and hence, by Liouville's theorem, constant. In fact, since

$$|\Gamma g(x)| \leq \frac{\|g\|_{L^1(\mathbb{R}^n)}}{s_n \cdot \operatorname{dist}(x, \operatorname{supp} g)^{n-2}}, \quad x \notin \operatorname{supp} g,$$

we see that $\Gamma g(x) \to 0$ as $|x| \to \infty$. Since also $w(x) \to 0$ as $|x| \to \infty$, the identity (1.2.6) follows. Now, for large $|x|$, we have $w(x) = (a/|x|)^{n-2}$ by Theorem 1.2.2. Comparing with (1.2.6) we see that

$$a^{n-2} = \frac{1}{2 s_n} \int_{\mathbb{R}^n} \left(\frac{|x|}{|x - y|} \right)^{n-2} g(y) \, dy,$$

for large $|x|$, and in the limit $|x| \to \infty$, the dominated convergence theorem then yields

$$2 s_n a^{n-2} = \int_{\mathbb{R}^n} g(y) \, dy. \tag{1.2.7}$$

Given any function $f \in L^1(\mathbb{R}^n)$ we let

$$\hat{f}_p = \hat{f}(p) := \int_{\mathbb{R}^n} e^{-ip \cdot x} f(x) \, dx$$

denote its Fourier transform. Note that if f is real and even, then $\hat{f}$ is real. We also note that if f is radially symmetric, then so is $\hat{f}$. The function w above is not in $L^1(\mathbb{R}^n)$, since $w(x) = (a/|x|)^{n-2}$ for large $|x|$. However, it follows from (1.2.5) that, as a tempered distribution, $\hat{w}$ equals the function $p \mapsto \hat{g}_p/(2p^2)$. We shall abuse notation slightly by denoting

$$\hat{w}_p := \frac{\hat{g}_p}{2p^2}.$$

By (1.2.7) we have

$$2s_n a^{n-2} = \hat{g}_0 = \hat{V}_0 - \hat{\varphi}_0. \tag{1.2.8}$$

Now notice that

$$\begin{aligned}\hat{\varphi}_p &= \frac{1}{(2\pi)^n}\int \hat{V}_{q-p}\hat{w}_q\,dq = \frac{1}{(2\pi)^n}\int \hat{V}_{q-p}\frac{\hat{g}_q}{2q^2}\,dq \\ &= \frac{1}{(2\pi)^n}\int \frac{\hat{V}_{q-p}\hat{V}_q}{2q^2}\,dq - \frac{1}{(2\pi)^n}\int \frac{\hat{V}_{q-p}\hat{\varphi}_q}{2q^2}\,dq.\end{aligned}$$

Using this iteratively and inserting into (1.2.8), we obtain the so-called Born series

$$2s_n a^{n-2} = \hat{V}_0 - \frac{1}{(2\pi)^3}\int \frac{\hat{V}_p^2}{2p^2}\,dp + \frac{1}{(2\pi)^6}\int\int \frac{\hat{V}_p\hat{V}_{q-p}\hat{V}_q}{4p^2q^2}\,dqdp - \dots$$

in terms of the Fourier transform of V.

1.3 Previous Works

The first systematic and semi-rigorous treatment of the 3-dimensional problem was by Bogoliubov in the 1940's [2] and Lee-Huang-Yang in the 1950's [9, 10]. In particular the latter used the so-called pseudo-potential method to derive the asymptotic expansion

$$e_0(\rho) = 4\pi a\rho\Big(1 + \frac{128}{15\sqrt{\pi}}Y^{1/2} + o\big(Y^{1/2}\big)\Big) \quad \text{as } Y \to 0,$$

now known as the Lee-Huang-Yang formula (LHY). Subsequently several other derivations of LHY appeared, but unfortunately none of them were rigorous [16]. The only rigorous result was the bounds

$$\frac{1}{10\sqrt{2}} \le \frac{e_0(\rho)}{4\pi a\rho} \le 1 + CY^{1/3} \quad (Y \text{ sufficiently small})$$

obtained by Dyson in 1957 [3]. Here $C > 0$ is a constant independent of V. While Dyson's upper bound is consistent with *the leading order term* in LHY, the lower bound is off the mark by a factor 1/14. It took more than 40 years before a matching leading order lower bound was proved. This was done by Lieb-Yngvason [14], who showed that

$$e_0(\rho) \ge 4\pi a\rho\big(1 - CY^{1/17}\big),$$

for Y sufficiently small, depending on V. Dyson actually only considered the hard-core potential, but his upper bound was later generalized to nonnegative, radially symmetric potentials [11]. Thus there is a rigorous proof of the leading order term in LHY:

Theorem 1.3.1 (Dyson/Lieb-Yngvason)**.** *Suppose that V is nonnegative, radially symmetric, measurable and integrable at infinity. Then*

$$e_0(\rho) = 4\pi a\rho\big[1 + o(1)\big] \quad \text{as } \rho \to 0.$$

The next problem is then to obtain a rigorous proof of the correction term in LHY. As we shall see below there has been success regarding an upper bound. However, for the matching lower bound there has only been limited progress. The method of Lieb-Yngvason has been improved by J.O. Lee and Yin in [8] to yield an error term of order $\rho^{1/3}|\ln\rho|^3$. Also, the result of Giuliani-Seiringer [6] shows that LHY is correct in a so-called simultaneously weak coupling and high density regime, and for a rather narrow class of potentials. But the general problem remains open.

Unfortunately it is not easy to improve Dyson's method directly. Instead it has turned out successful to pass to momentum space (see Chapter 2). In [4] a trial state of the form

$$\Psi = \exp\left(\frac{1}{2}\sum_{p\neq 0} c_p a_p^+ a_{-p}^+ + \sqrt{N_0}a_0^+\right)|0\rangle \tag{1.3.1}$$

was used to derive the following upper bound:

Theorem 1.3.2 (Erdős-Schlein-Yau 2008)**.** *Suppose that $\tilde{V}$ is nonnegative, radially symmetric and smooth with a decay $\tilde{V}(x) \le C(1+|x|)^{-(3+\delta)}$, for some $\delta > 0$. Let $\lambda > 0$ be small and set $V = \lambda\tilde{V}$. Then*

$$e_0(\rho) \le 4\pi a\rho\left(1 + \frac{128}{15\sqrt{\pi}}(1 + C\lambda)Y^{1/2}\right) + \mathcal{O}(\rho^2|\ln\rho|) \quad \text{as } \rho \to 0. \tag{1.3.2}$$

Here a is the scattering length of V, while $C > 0$ is independent of V.

We see that the second order term in (1.3.2) has the correct order in Y, but the constant is only correct in the limit of weak coupling, $\lambda \to 0$. The trial state (1.3.1) is inspired by the Bogoliubov approximation (Section 2.1), and its crucial feature is that particles of nonzero momenta appear only in *pairs* of opposite momenta $p, -p$. A similar state was used by Girardeau and Arnowitt in [5] in the context of a Bose gas, only here the energy was not evaluated explicitly. We also note that the approach in [4] has the advantage over [5] that (1.3.1) is considered in a grand canonical ensemble. This is a technical convenience which simplifies some of the calculations.

A trial state of the form (1.3.1) is in general believed to yield the energy of LHY, and the result of Theorem 1.3.2 above may at first sight appear to be close enough to the desired to be repaired. This is not so easy though! In [4] the energy in the state Ψ is calculated in terms of (integrals of various combinations of) the c_p's, and the task is then to make the best possible choice of these coefficients. Unfortunately, this choice is not obvious and a compromise must be taken. The strategy of [4] is to declare the main terms in consistency with the Bogoliubov approximation, and then a posteriori justify that the neglected terms are indeed of lower order in the energy. Finally, the energy of the main terms is calculated explicitly (in the dilute limit) and the result is the right-hand-side of (1.3.2). It is an interesting question whether one could make a better choice of the c_p's e.g. by taking some of the neglected terms in consideration also. Nevertheless we want to point out the following: A trivial upper bound to $e_0(\rho)$ can be obtained by calculating the energy of the constant function,

$$e_0(\rho) \leq \frac{1}{2}\Big(\int_{\mathbb{R}^3} V(x)\,dx\Big)\rho.$$

The integral here is the first term in the Born approximation to $8\pi a$, and one can easily show that for a coupled potential $V = \lambda\tilde{V}$, we then have

$$e_0(\rho) \leq 4\pi a(1 + C\lambda)\rho.$$

The point is that, to get rid of the term $C\lambda$, we clearly have to consider a more general trial state. This suggests that one really has to 'do more' than (1.3.1) in order to capture the correct constant in LHY. The challenge was taken up by Yau and Yin in their paper [25] from 2009. They introduced a new type of trial state, extending the properties of (1.3.1). More precisely, they include pairs with total momentum of order $\rho^{1/2}$, the so-called *soft-pair's*. This produces additional terms in the energy, and their result is an upper bound consistent with LHY:

Theorem 1.3.3 (Yau-Yin 2009)**.** *Suppose that V is nonnegative, radially symmetric and smooth with fast decay. Suppose furthermore that V is sufficiently small for the Born series to converge. Then*

$$\limsup_{\rho\to 0}\left(\frac{e_0(\rho) - 4\pi a\rho}{(4\pi a)^{5/2}\rho^{3/2}}\right) \leq \frac{16}{15\pi^2}.$$

The proof of theorem 1.3.3 as it appears in [25] is severely complicated compared to the proof of Theorem 1.3.2 in [4]. The reason is mainly two-fold: Firstly, the trial state of [25] is more general, as it should be. Consequently there are more terms in the energy to be estimated, and some of the nice symmetry properties of (1.3.1) do not apply. Secondly, the trial state of [25] has a fixed number of particles, in contrast to [4].

Having discussed 3-dimensional results, we now turn briefly to other dimensions. The one-dimensional case with a delta-function potential was considered by Lieb-Liniger in [12] and turned out to be exactly solvable. In 2 dimensions the leading order term was, to our knowledge, first identified by Schick [20] in 1971 to be $4\pi\rho|\ln Y|^{-1}$. This was rigorously proven to be correct by Lieb-Yngvason in 2001 [15]. To our knowledge there are yet no rigorous results on the 2-dimensional correction term (in fact, it seems that there is not even complete consensus about what this term should be: compare e.g. [20], [24] and [17]). In [24] Yang reexamined the pseudo-potential method in dimension 2, 4 and 5. In the latter he found the method inconclusive, while he in four dimensions derived the expansion

$$e_0(\rho) = 4\pi^2 a^2\rho\big[1 + 2\pi^2 Y|\ln Y| + o\big(Y\ln Y\big)\big] \quad \text{as } Y \to 0. \tag{1.3.3}$$

We remark that in Yangs paper the correction $2\pi^2 Y|\ln Y|$ appears to be $4\pi^2 Y|\ln Y|$, due to a minor miscalculation.

1.4 Outline

In Chapter 2 we describe in more detail some of the tools applied in the subsequent chapters. Also, we explain the Bogoliubov approximation and show how it leads to LHY. In particular this will motivate the ansatz in (1.3.1).

In Chapter 3 we consider the Bose gas in arbitrary dimension $n > 3$. We first follow the proofs of Dyson and Lieb-Yngvason and obtain n-dimensional upper and lower bounds to $e_0(\rho)$ (Theorem 3.2.2, Theorem 3.2.3 and Corollary 3.2.10). As a consequence we get the following n-dimensional analogue of Theorem 1.3.1 above.

Theorem 1.4.1. *Let $n \geq 3$ and suppose that V is nonnegative, radially symmetric, measurable and decays faster than $r^{-\nu}$ at infinity, where $\nu = (6n-2)/5$. Suppose furthermore that V admits a scattering solution. Then*

$$e_0(\rho) = s_n a^{n-2}\rho\big[1 + o(1)\big] \quad \text{as } \rho \to 0.$$

Next we employ the trial state in (1.3.1) to obtain the following second order upper bounds.

Theorem 1.4.2. *Let $n \geq 3$ and suppose that V is nonnegative, radially symmetric, smooth and compactly supported with $V(0) > 0$. In dimension $n = 4$,*

$$e_0(\rho) \leq 4\pi^2 a^2 \rho\big[1 + 2\pi^2(1+\gamma)Y|\ln Y|\big] + \mathcal{O}(\rho^2) \quad \text{as } \rho \to 0,$$

where $0 < \gamma \leq C\|V\|_\infty^{1/2}\|V\|_1^{1/2}$. In dimension $n \geq 5$,

$$e_0(\rho) \leq s_n a^{n-2}\rho + \mathcal{O}(\rho^2) \quad \text{as } \rho \to 0.$$

The second order asymptotics of $e_0(\rho)$ becomes more subtle in dimension $n > 3$. The correction to the energy is given in terms of certain integrals, which, in three dimensions, are exactly computable in the limit $\rho \to 0$, in a straight-forward manner. This is not the case in higher dimensions, and a more careful analysis has to be carried out. In dimension $n \geq 5$ we have not even been able to identify the expansion parameter Y in the correction term, nor an explicit coefficient. Chapter 3 (except Appendix 3.B) is submitted as a paper. We have included it here in its submitted form, and hence there will be minor repetitions from Chapter 1 and Chapter 2.

In Chapter 4 we consider the Bose gas in dimension 3 and 4. We carry out a grand canonical calculation of the energy in the Yau-Yin trial state from [25]. In 3 dimensions this yields a substantially simpler proof of the upper bound in Theorem 1.3.3 compared to [25]. In fact, we show the following slightly stronger upper bound.

Theorem 1.4.3. *Let $n = 3$ and suppose that V is nonnegative, radially symmetric, smooth and compactly supported with $V(0) > 0$. Let $0 < \eta < 1/52$. Then*

$$e_0(\rho) \leq 4\pi a\rho\left(1 + \frac{128}{15\sqrt{\pi}}Y^{1/2}\right) + \mathcal{O}\big(\rho^{\frac{3}{2}+\eta}\big) \quad \text{as } \rho \to 0.$$

In 4 dimensions, unfortunately, the method does not apply. We have included the calculations though, and we will explain in detail the reason for this break down.

1.A Proof of Theorem 1.2.2

The proof given here is a somewhat modified version of the one found in Appendix A in [15]. Recall that $n \geq 3$ and $s_n := (n-2)|\mathbb{S}^{n-1}|$. We start by noting that any radially symmetric function $u \in H^1_{\text{loc}}(\mathbb{R}^n)$ is continuous away from the origin. Indeed if, say, $r > r_0 > 0$, then, by the fundamental theorem of calculus,

$$\begin{aligned} |u(r) - u(r_0)| &\leq \int_{r_0}^{r} |u'(t)|\, dt \leq \frac{1}{r_0^{n-1}} \int_{r_0}^{r} |u'(t)| t^{n-1}\, dt \\ &= \frac{1}{r_0^{n-1}|\mathbb{S}^{n-1}|} \int_{r_0 \leq |x| \leq r} |\nabla u(x)|\, dx, \end{aligned} \tag{1.A.1}$$

and the last quantity can be made arbitrarily small, by taking r sufficiently close to r_0.

Suppose that $\operatorname{supp}(V) \subset B(0, R_0)$ and fix and arbitrary $R > R_0$. Let $B = B(0, R)$ and define the auxiliary functional $\mathcal{E} = \mathcal{E}_R$ by

$$\mathcal{E}(u) = \int_B |\nabla u|^2 + \frac{1}{2} V |u|^2$$

on the set $\mathcal{D} := \{u \in H^1(B) :\ u = 1 \text{ on } \partial B\}$. Let $E := \inf_{u \in \mathcal{D}} \mathcal{E}(u)$. We claim that $\mathcal{E}$ has a nonnegative, radially symmetric minimizer $u \in \mathcal{D}$. To show this, choose a minimizing sequence $\{u_k\} \in \mathcal{D}$ such that $\mathcal{E}(u_k) \to E$. In particular the sequence $\mathcal{E}(u_k)$ is bounded and, since V is nonnegative, ∇u_k is bounded in $L^2(B)$. Moreover, since $(u_k - 1) \in H^1_0(B)$, the Poincaré inequality yields

$$\|u_k\|_{L^2(B)} \leq \|u_k - 1\|_{L^2(B)} + |B|^{1/2} \leq C \|\nabla u_k\|_{L^2(B)} + |B|^{1/2},$$

and hence u_k is bounded in $H^1(B)$. By the Banach-Alaoglu theorem there exists a $u \in H^1(B)$ and a subsequence, also denoted by u_k, such that $u_k \rightharpoonup u$ weakly in $H^1(B)$. Since $H^1(B)$ is compactly embedded in $L^2(B)$, we may assume that $u_k \to u$ in $L^2(B)$ and consequently also that $u_k \to u$ a.e. Since $\mathcal{D}$ is a closed and convex subset of $H^1(B)$ it follows, by Mazur's Theorem, that $\mathcal{D}$ is weakly closed and hence $u \in \mathcal{D}$. Finally, by weak lower semicontinuity of the L^2-norm and Fatou's Lemma, we see that

$$E = \liminf_{k \to \infty} \mathcal{E}(u_k) \geq \|\nabla u\|^2_{L^2(B)} + \frac{1}{2} \int_B \liminf_{k \to \infty} V |u_k|^2 = \mathcal{E}(u),$$

and hence u is a minimizer. Since $|u| \in \mathcal{D}$ and $\mathcal{E}(|u|) \leq \mathcal{E}(u)$, we may assume that u is nonnegative. Moreover, we can assume that u is radial. To see this consider the function

$$u_s(x) := \int_{\mathbb{S}^{n-1}} u(|x|\omega)\, d\mu(\omega),$$

where μ denotes the normalized surface measure on $\mathbb{S}^{n-1}$. By passing into polar coordinates it is evident that $\|u_s\|_{L^2(B)} \leq \|u\|_{L^2(B)}$ and

$$\int_B V u_s^2 \leq \int_B V u^2.$$

Moreover, an approximation argument employing the fact that $\mathcal{D} \cap C^1(\bar{B})$ is dense in $\mathcal{D}$ and that $\mathcal{D}$ is closed, shows that $u_s \in \mathcal{D}$ with

$$\nabla u_s(x) = \int_{\mathbb{S}^{n-1}} \left[\nabla u(|x|\omega) \cdot \omega\right] \frac{x}{|x|} \, d\mu(\omega), \quad \text{for } x \neq 0. \tag{1.A.2}$$

It follows that $\|\nabla u_s\|_{L^2(B)} \leq \|\nabla u\|_{L^2(B)}$, and hence $\mathcal{E}(u_s) \leq \mathcal{E}(u)$. We continue by establishing further properties of u.

1. u is radially increasing. Suppose that $0 < s < t \leq R$ and $u(s) > u(t)$. Choose $\tau \in (s, t]$ such that $u(\tau) \leq u(r)$ for all $r \in [s, t]$. Then define the radial function

$$v(r) = \begin{cases} \min\{u(\tau), u(r)\} & \text{for } 0 \leq r \leq \tau \\ u(r) & \text{for } r > \tau \end{cases}.$$

Then $v \in \mathcal{D}$ and

$$\mathcal{E}(u) - \mathcal{E}(v) \geq s_n \int_s^\tau u'(r)^2 r^{n-1} \, dr > 0,$$

since otherwise $u' = 0$ a.e. on $[s, \tau]$ and consequently

$$u(\tau) - u(s) = \int_s^\tau u'(r) \, dr = 0.$$

However, $\mathcal{E}(v) < \mathcal{E}(u)$ contradicts the fact that u is a minimizer.

2. u is continuous. Since u is in $H^1(B)$ and is radial, it is continuous away from the origin by the argument in (1.A.1). However, since u is increasing and bounded from below, it can be chosen to be continuous at the origin also.

3. u is the only nonnegative, radial minimizer. Suppose that also v is a nonnegative, radial minimizer (which by the above is continuous and radially increasing). The function $w := \sqrt{u^2 + v^2}$ is in $H^1(B)$ with

$$\nabla w = \frac{(u\nabla u + v\nabla v)\chi_E}{\sqrt{u^2 + v^2}},$$

where $E := \{x \in B : u(x)^2 + v(x)^2 > 0\}$. A direct computation shows that

$$\int_B |\nabla w|^2 + \int_E \frac{|v\nabla u - u\nabla v|^2}{u^2 + v^2} = \int_B |\nabla u|^2 + \int_B |\nabla v|^2$$

and, since $(w/\sqrt{2}) \in \mathcal{D}$ and $\mathcal{E}(v) = \mathcal{E}(u)$, it follows that

$$\mathcal{E}(u) \leq \mathcal{E}(w/\sqrt{2}) = \mathcal{E}(u) - \frac{1}{2} \int_E \frac{|v\nabla u - u\nabla v|^2}{u^2 + v^2}.$$

Consequently

$$v\nabla u = u\nabla v \quad \text{a.e. on } E. \tag{1.A.3}$$

Fix $0 < \varepsilon < 1$ and let $A = \{x \in B : u(x) > \varepsilon\}$. If $A \neq B$ then A is an open annulus, since u is radially increasing and continuous. Now choose an arbitrary test function $\varphi \in C_0^\infty(A)$, and let $h = \varphi/u$. Then $h \in H^1(A)$ with

$$\nabla h = \frac{(\nabla\varphi)u - \varphi\nabla u}{u^2}.$$

By (1.A.3) and an integration by parts (using that h vanishes on ∂A), we get

$$\int_A v\nabla h = \int_A \frac{v}{u}\nabla\varphi - \int_A h\nabla v = \int_A \frac{v}{u}\nabla\varphi + \int_A v\nabla h,$$

and hence

$$\int_A \frac{v}{u}\nabla\varphi = 0. \tag{1.A.4}$$

Since (1.A.4) holds for any $\varphi \in C_0^\infty(A)$, it follows that v/u is constant on A, and the boundary conditions then yields $u = v$ on A. We may take ε arbitrary small, so we conclude that $u = v$ whenever $u > 0$. Finally, we of course also have $u = v$ whenever $v > 0$, and hence $u = v$.

4. u satisfies $-\Delta u + \frac{1}{2}Vu = 0$ in the sense of distributions on B. Notice that $V \in L^1(B)$ by assumption, and hence Vu is indeed a distribution. Fix an arbitrary $v \in C_0^\infty(B)$. We need to show that

$$\int_B -u\Delta v + \frac{1}{2}Vuv = 0. \tag{1.A.5}$$

For each $t \in \mathbb{R}$ we have $(u + tv) \in \mathcal{D}$ and

$$\mathcal{E}(u + tv) = \mathcal{E}(u) + t^2\mathcal{E}(v) + t \cdot \mathrm{Re}\int_B \nabla u \cdot \nabla v + \frac{1}{2}vuv$$

Since u minimizes $\mathcal{E}$,

$$0 = \frac{d}{dt}\mathcal{E}(u + tv)\big|_{t=0} = \mathrm{Re}\int_B \nabla u \cdot \nabla v + \frac{1}{2}Vuv = \mathrm{Re}\int_B -u\Delta v + \frac{1}{2}Vuv,$$

where the last equality follows from integration by parts and by noting that v (and derivatives of v) vanishes on ∂B. Replacing v with $-iv$ we find that the imaginary part of the above integral vanishes and hence (1.A.5) holds.

5. Since u is radial and harmonic in $R_0 < |x| < R$, and since $u(R) = 1$, it follows that

$$u(r) = u^{\mathrm{as}}(r) := \frac{1 - (\alpha/r)^{n-2}}{1 - (\alpha/R)^{n-2}}, \qquad R_0 \le r \le R,$$

for some number $\alpha \ge 0$. Note that, in case $\alpha = 0$, we have $u = 1$ on $R_0 \le |x| \le R$, and hence u attains its maximum in an interior point of $B(0, R)$. From the scattering equation and the fact that V is nonnegative it follows that u is subharmonic, and hence u is constant. However, this implies that $V = 0$.

6. $u(r) \ge u^{\mathrm{as}}(r)$ for all $0 < r \le R$. Suppose that $u(\rho) < u^{\mathrm{as}}(\rho)$, for some $0 < \rho < R_0$. For $\varepsilon > 0$ we define

$$h_\varepsilon(r) = 2\big(u(r) - (1 + \varepsilon)u^{\mathrm{as}}(r)\big), \quad 0 < r \le R,$$

Notice that $h_\varepsilon(r) = -2\varepsilon u^{\mathrm{as}}(r)$, for $r \ge R_0$, and in particular $h_\varepsilon(R) = -2\varepsilon$. Also, h_ε is strictly decreasing on $[R_0, R]$ (if $V \ne 0$) and hence $h_\varepsilon(R_0) > -2\varepsilon$. By the particular choice of

$$\varepsilon = \frac{u^{\mathrm{as}}(\rho) - u(\rho)}{1 - u^{\mathrm{as}}(\rho)},$$

we obtain $h_\varepsilon(\rho) = -2\varepsilon$. Now let $\Omega = \{x \in \mathbb{R}^n : \rho < |x| < R\}$. Since u^{as} is harmonic, it follows that h_ε is subharmonic on Ω and, by the maximum principle,

$$\max_{\bar{\Omega}} h_\varepsilon = \max_{\partial\Omega} h_\varepsilon = -2\varepsilon,$$

which contradicts the fact that $h_\varepsilon(R_0) > -2\varepsilon$.

7. Employing 4. and 5., an integration by parts yields

$$\mathcal{E}(u) = s_n \alpha^{n-2}\big[1 - (\alpha/R)^{n-2}\big]^{-1}.$$

8. If $\tilde{R} > R$ and u, $\tilde{u}$ denotes the corresponding minimizers of $\mathcal{E}_R$ and $\mathcal{E}_{\tilde{R}}$ respectively, then

$$\tilde{u}(r) = \tilde{u}(R)u(r), \quad \text{for } r \leq R,$$

which in particular shows that α is independent of R. To verify this define

$$v(r) = \begin{cases} \tilde{u}(R)u(r), & 0 \leq r \leq R \\ \tilde{u}(r), & R < r \leq \tilde{R} \end{cases}$$

Since

$$\mathcal{E}_R(u) \leq \mathcal{E}_R\big(\tilde{u}/\tilde{u}(R)\big) = \tilde{u}(R)^{-2}\mathcal{E}_R(\tilde{u}),$$

we get

$$\mathcal{E}_{\tilde{R}}(v) = \tilde{u}(R)^2\mathcal{E}_R(u) + \int_{B_{\tilde{R}}\setminus B_R} |\nabla\tilde{u}|^2 + \frac{1}{2}V|\tilde{u}|^2 \leq \mathcal{E}_{\tilde{R}}(\tilde{u})$$

and, by uniqueness, we must have $v = \tilde{u}$, as desired.

To summarize: for each $R > R_0$ we have a minimizer u_R of the functional $\mathcal{E}_R$ with the properties 1.-8. We can easily obtain the desired minimizer u of the functional in (3.2.1). Simply let

$$u(r) = \big[1 - (\alpha/R)^{n-2}\big]u_R(r) \quad \text{for } r \leq R,$$

where $C_R := \big[1 - (\alpha/R)^{n-2}\big]$. By 8. u is well-defined. Fix an arbitrary nonnegative, radial function $v \in H^1_{\text{loc}}(\mathbb{R}^n)$ satisfying $v(r) \to 1$ as $r \to \infty$. Since $C_R^{-1}u$ minimizes $\mathcal{E}_R$, we get

$$\mathcal{E}_R(u) = C_R^2\mathcal{E}_R(u_R) \leq C_R^2\mathcal{E}_R(v/v(R)) = C_R^2/v(R)^2\mathcal{E}_R(v),$$

and by taking the limit as $R \to \infty$, it follows that

$$s_n a^{n-2} = \int_{\mathbb{R}^n} |\nabla u|^2 + \frac{1}{2}V|u|^2$$

On the other hand 7. implies that

$$\mathcal{E}_R(u) = C_R^2\mathcal{E}_R(u_R) = C_R s_n \alpha^{n-2},$$

and letting $R \to \infty$, we conclude that $\alpha = a$. The remaining properties of u are easily obtained from the corresponding properties of the minimizers of $\mathcal{E}_R$.

Chapter 2

Momentum Space Representation

In this chapter we describe the important idea of considering the Hamiltonian in momentum space. It was this representation that led Bogoliubov to his famous approximation, which we also explain here. In particular we will motivate the Lee-Huang-Yang formula and see how the Bogoliubov approximation leads to the ansatz in (1.3.1).

A standard trick in many-body quantum mechanics is to pass to the grand canonical ensemble. Thus we introduce the bosonic Fock (Hilbert) space

$$\mathcal{F} = \mathcal{F}_L(\mathcal{H}) := \bigoplus_{N=0}^{\infty} \mathcal{H}_N^{\mathrm{sym}} \quad (\mathcal{H}_0^{\mathrm{sym}} = \mathcal{H}_0 := \mathbb{C}).$$

The special vector $|0\rangle := (1, 0, 0, \ldots)$ is called the *vacuum*. Operators on N-particle spaces can then be lifted, or second quantized, to densely defined operators on the Fock space by a componentwise action. We let

$$H_L := \bigoplus_{N=0}^{\infty} H_{N,L} \quad (H_{0,L} := 0) \tag{2.0.1}$$

denote the second quantization of $H_{N,L}$ from (1.1.3). We furthermore let $\mathcal{N} = \mathcal{N}_L$ denote the second quantization of multiplication with N on $\mathcal{H}_N$, i.e.

$$\mathcal{N}\Psi := \bigoplus_{N=0}^{\infty} N\Psi_N.$$

$\mathcal{N}$ is called the *number operator* on $\mathcal{F}$. Now, the obvious question is how to retrieve information about $e_0(\rho)$ from this grand canonical setting. To answer this, we define the 'grand canonical ground state energy'

$$E_0^{\mathrm{GC}}(N, L) := \inf \left\{ \langle H_L \rangle_\Psi : \|\Psi\| = 1,\, \langle \mathcal{N} \rangle_\Psi \geq N \right\}. \tag{2.0.2}$$

Here $\langle \cdot \rangle_\Psi := \langle \Psi, \cdot \Psi \rangle_{\mathcal{F}}$ denotes the expectation value w.r.t. the inner product of the Fock space. In Appendix 3.A we prove the following result, provided Dirichlet boundary conditions are imposed. Of course, since the statement in the lemma concerns only the thermodynamic limit, we expect it to hold for other boundary conditions as well.

Lemma 2.0.1. *Suppose that $V \in L^1(\mathbb{R}^n)$ is nonnegative, radially symmetric and compactly supported. Suppose furthermore that $V \geq \varepsilon \chi_{B(0,2R)}$, for some $\varepsilon, R > 0$. Then*

$$e(\rho) = \lim_{L\to\infty} \frac{E_0^{GC}(\rho L^n, L)}{\rho L^n}.$$

We remark that Lemma 2.0.1 remains true if the condition $\langle \mathcal{N} \rangle_\Psi \geq N$ in (2.0.2) is replaced by $\langle \mathcal{N} \rangle_\Psi = N$, which might appear more natural. The idea of the proof of Lemma 2.0.1 is to relate the canonical ground state energy to the grand canonical ground state energy via the Legendre transform. In order for the latter to be well-defined globally, we need high-density bounds on $e_0(\rho)$. It is at this point we need the assumption $V \geq \varepsilon \chi_{B(0,2R)}$. Of course, if V is continuous, then $V(0) > 0$ suffices, and hence this condition is imposed in the relevant theorems in the subsequent chapters.

Returning to the N-particle space in (1.1.1), we define the *symmetrization* P_{sym} initially on pure tensors in $\mathcal{H}_N$ by

$$P_{\mathrm{sym}}(f_1 \otimes \cdots \otimes f_N) = \frac{1}{N!} \sum_{\sigma \in S_N} f_{\sigma(1)} \otimes \cdots \otimes f_{\sigma(N)},$$

where S_N denotes the symmetric group of permutations of the numbers $1, \ldots, N$. Then P_{sym} extends to a bounded operator on $\mathcal{H}_N$ in the usual way, and in fact it is an orthogonal projection. The symmetric space is then

$$\mathcal{H}_N^{\mathrm{sym}} = P_{\mathrm{sym}}(\mathcal{H}_N).$$

Given any $f \in \mathcal{H}$ we define the *creation operator* $a^*(f) : \mathcal{H}_N \to \mathcal{H}_{N+1}$ by

$$a^*(f)\Psi = \sqrt{N+1} f \otimes \Psi.$$

The adjoint of $a^*(f)$ is the operator $a(f) : \mathcal{H}_{N+1} \to \mathcal{H}_N$ satisfying

$$\langle \Phi, a^*(f)\Psi \rangle = \langle a(f)\Phi, \Psi \rangle, \quad \text{for each } \Phi \in \mathcal{H}_{N+1} \text{ and } \Psi \in \mathcal{H}_N.$$

We call $a(f)$ the *annihilation operator*. It easily follows that

$$a(f)(g \otimes \Psi) = \sqrt{N+1} \langle f, g \rangle \Psi$$

for any $g \in \mathcal{H}$ and $\Psi \in \mathcal{H}_N$. More importantly we define the *bosonic* creation and annihilation operators

$$a_{\mathrm{sym}}(f) = a(f) \quad \text{and} \quad a^*_{\mathrm{sym}}(f) = P_{\mathrm{sym}} a^*(f)$$

on the symmetric spaces $\mathcal{H}_N^{\mathrm{sym}}$. We remark that $a(f)$ automatically maps a symmetric space into a symmetric space. This is not the case for $a^*(f)$ and hence we need to compose with the symmetrization. The bosonic creation an annihilation operators are also the adjoint of one another and furthermore, they satisfy the canonical commutation relations (CCR):

$$\left[a_{\mathrm{sym}}(f), a_{\mathrm{sym}}(g)\right] = 0 = \left[a^*_{\mathrm{sym}}(f), a^*_{\mathrm{sym}}(g)\right] \quad \text{and} \quad \left[a_{\mathrm{sym}}(f), a^*_{\mathrm{sym}}(g)\right] = \langle f, g \rangle I,$$

where $[A, B] := AB - BA$ is the commutator of A with B, and where I denotes the identity. We will apply the above general construction in a special setting. Let

$$\Lambda^* = \Lambda_L^* := (2\pi/L)\mathbb{Z}^n.$$

For each $p \in \Lambda^*$ we let $u_p(x) = L^{-n/2}e^{ip\cdot x}$, for $x \in \mathbb{R}^n$. The set $\{u_p : p \in \Lambda^*\}$ is an orthonormal basis in $\mathcal{H} = L^2(\Lambda)$. To keep notation simple we set

$$a_p := a_{\text{sym}}(u_p) \quad \text{and} \quad a_p^+ := a_{\text{sym}}^*(u_p).$$

The CCR then takes the form

$$[a_p, a_q] = 0 = [a_p^+, a_q^+] \quad \text{and} \quad [a_p, a_q^+] = \delta_{p,q}.$$

Now, suppose that $V, \hat{V} \in L^1(\mathbb{R}^n)$ with a decay

$$|V(x)| + |\hat{V}(x)| \leq C(1 + |x|)^{-(n+\varepsilon)},$$

for some $C, \varepsilon > 0$. Then the L-periodization of V exists and the Poisson summation formula holds [7]:

$$V_L(x) := \sum_{m\in\mathbb{Z}^n} V(x + mL) = \frac{1}{L^n} \sum_{p\in\Lambda_L^*} \hat{V}_p e^{ip\cdot x}, \quad x \in \mathbb{R}^n. \tag{2.0.3}$$

Note that

$$\lim_{L\to\infty} V_L(x) = \frac{1}{(2\pi)^n} \int e^{ip\cdot x}\hat{V}_p \, dp = V(x) \tag{2.0.4}$$

by Fourier's inversion formula. Suppose furthermore that V is nonnegative and radially symmetric. Then consider

$$H_{N,L}^{\text{per}} := \sum_{i=1}^{N} -\Delta_i + \sum_{1\leq j<k\leq N} V_L(x_j - x_k) \tag{2.0.5}$$

with periodic boundary conditions and let $\tilde{e}_0(\rho)$ denote the corresponding ground state energy per particle in the thermodynamic limit. Since V is nonnegative, it is clear that $V \leq V_L$ and consequently $e_0(\rho) \leq \tilde{e}_0(\rho)$. However, due to the convergence in (2.0.4), we expect that $e_0(\rho) = \tilde{e}_0(\rho)$. With the periodic potential V_L one can show that in the sense of quadratic forms [23],

$$H_{N,L}^{\text{per}} = \sum_p p^2 a_p^+ a_p + \frac{1}{2|\Lambda|} \sum_{\substack{p,q,r,s \\ p+q=r+s}} \hat{V}_{p-r} a_p^+ a_q^+ a_r a_s, \tag{2.0.6}$$

where all sums are over Λ^*, and where the original potential V reappears in terms of its Fourier transform.

The creation and annihilation operators defined above do not preserve particle numbers, e.g. a_p maps from $\mathcal{H}_N$ into $\mathcal{H}_{N-1}$. One particular advantage of passing to the grand canonical ensemble is that the second quantization of the creation and annihilation operators (which we also denote by a_p and a_p^+) are operators from $\mathcal{F}$ into itself. Moreover, a_p^+ is still the (formal) adjoint of a_p and the CCR, as well as the representation (2.0.6), remain valid on a dense subset of $\mathcal{F}$. Before we discuss the Bogoliubov approximation we will illustrate how the grand canonical ground state of the non-interacting system can be represented in terms of creation operators. Let

$$\Psi_0 = \exp\big(\sqrt{N_0}a_0^+\big)|0\rangle := \sum_{m=0}^{\infty} \frac{(\sqrt{N_0}a_0^+)^m}{m!}|0\rangle. \tag{2.0.7}$$

By employing the CCR it is easy to see that

$$\langle \Psi_0, \Psi_0\rangle = e^{N_0} \quad \text{and} \quad \langle \Psi_0, \mathcal{N}\Psi_0\rangle = N_0.$$

Furthermore, it also clear that $a_p\Psi_0 = 0$, for each $p \neq 0$. Thus, if we take $N_0 = \rho|\Lambda|$ and then normalize, we have the grand canonical ground state of the non-interacting Bose gas.

2.1 The Bogoliubov Approximation

The partially heuristic presentation given here follows [5, 16] rather closely. Consider $H = H_L^{\text{per}}$ (the second quantization of (2.0.5)) on the set of normalized Fock states Ψ with an expected number of particles $\langle \mathcal{N}\rangle_\Psi = N := \rho|\Lambda|$. Bogoliubov's way of thinking of the dilute (and hence weakly interacting) Bose gas goes as follows: The ground state of the noninteracting system is given in (2.0.7). In this state all particles are in the condensate, i.e. have momentum zero. 'Turning on' the weak interaction, still the vast majority of the particles are in the condensate, while a small amount of particle pairs with equal and opposite momenta are created from the condensate. Only from particle pairs, the other groups of particles, i.e. double pairs, triples and quartets, can be created. Bogoliubov then proposes (the first ansatz) to discard all terms higher than quadratic in a_p and a_p^+, for $p \neq 0$. Since the expected number of particles in the condensate is given by the expectation of $a_0^+a_0$, Bogoliubov furthermore proposes (the second ansatz) to replace the operators a_0 and a_0^+ by $\sqrt{N}$. The resulting operator is

$$H^{\text{Bog}} := \frac{\hat{V}_0}{2}\rho(N-1) + \sum_{p\neq 0}\big(p^2 + \rho\hat{V}_p\big)a_p^+a_p + \frac{1}{2}\rho\hat{V}_p\big(\alpha_p + \alpha_p^+\big),$$

where $\alpha_p := a_p a_{-p}$. This operator can be diagonalized by a Bogoliubov transformation $\exp\big(F\big)$, where

$$F = \frac{1}{2}\sum_{p\neq 0}\gamma_p\big(\alpha_p - \alpha_p^+\big)$$

and $\gamma : \Lambda^*\backslash\{0\} \to \mathbb{R}$ is some even function to be chosen appropriately. Note that iF is self-adjoint, and hence $\exp\big(F\big)$ is unitary. We define the new 'creation and annihilation operators'

$$b_p := e^F a_p e^{-F} \quad \text{and} \quad b_p^+ = e^F a_p^+ e^{-F}.$$

Since $\exp\big(F\big)$ is unitary, the b_p's also satisfy the CCR. Now, we claim that

$$b_p = a_p\cosh\gamma_p + a_{-p}^+\sinh\gamma_p. \tag{2.1.1}$$

To show this we introduce

$$a_p(\varepsilon) := e^{\varepsilon F} a_p e^{-\varepsilon F}, \quad \varepsilon \in \mathbb{R}.$$

Taking (formally) derivative w.r.t. ε we obtain

$$\frac{da_p}{d\varepsilon}(\varepsilon) = F e^{\varepsilon F} a_p e^{-\varepsilon F} - e^{\varepsilon F} a_p F e^{-\varepsilon F} = [F(\varepsilon), a_p(\varepsilon)],$$

where $F(\varepsilon) := e^{\varepsilon F} F e^{-\varepsilon F}$, and where we have also used that F commutes with $e^{\varepsilon F}$ in the last equality. We continue to calculate

$$\begin{aligned}
[F(\varepsilon), a_p(\varepsilon)] &= e^{\varepsilon F}[F, a_p] e^{-\varepsilon F} \\
&= \frac{1}{2} e^{\varepsilon F} \left(\gamma_p [a_p, \alpha_p^+] + \gamma_{-p} [a_p, \alpha_{-p}^+] \right) e^{-\varepsilon F} \\
&= \gamma_p a_{-p}^+(\varepsilon),
\end{aligned}$$

where we have employed the commutator identity $[A, BC] = [A, B]C + B[A, C]$, the CCR and $\gamma_{-p} = \gamma_p$ to obtain the last equality. Thus we have

$$\frac{da_p}{d\varepsilon}(\varepsilon) = \gamma_p a_{-p}^+(\varepsilon).$$

Since differentiation commutes with complex conjugation, it then follows that

$$\frac{d^2 a_p}{d\varepsilon^2}(\varepsilon) = \gamma_p^2 a_p(\varepsilon).$$

The general solution to this ODE is

$$a_p(\varepsilon) = A_p \cosh(\gamma_p \varepsilon) + B_p \sinh(\gamma_p \varepsilon),$$

and the boundary condition $a_p(0) = a_p$ yields $A_p = a_p$, while

$$\gamma_p a_{-p}^+ = \gamma_p a_{-p}^+(0) = \frac{da_p}{d\varepsilon}(0) = \gamma_p B_p.$$

This verifies (2.1.1). By choosing

$$\tanh(2\gamma_p) = \frac{\rho \hat{V}_p}{p^2 + \rho \hat{V}_p},$$

it follows from a lengthy, but straight forward, calculation that

$$H^{\text{Bog}} = E_0^{\text{Bog}} + \sum_{p \neq 0} \left(p^4 + 2\rho p^2 \hat{V}_p \right)^{1/2} b_p^+ b_p,$$

where

$$E_0^{\text{Bog}} := \frac{\hat{V}_0}{2} \rho(N-1) + \frac{1}{2} \sum_{p \neq 0} p^2 \left[\left(1 + \frac{2\rho \hat{V}_p}{p^2} \right)^{1/2} - 1 - \frac{\rho \hat{V}_p}{p^2} \right].$$

Since $b_p^+ b_p$ is a nonnegative operator, it is now clear the (non-normalized) ground state of H^{Bog} is

$$\Psi^{\mathrm{Bog}} = e^F \Psi_0,$$

with Ψ_0 given in (2.0.7), and the ground state energy is then simply E_0^{Bog}. In the thermodynamic limit we have (replacing sums with integrals)

$$\begin{aligned} e_0^{\mathrm{Bog}}(\rho) &:= \lim_{L\to\infty} \frac{E_0^{\mathrm{Bog}}}{\rho L^n} \\ &= \frac{\hat{V}_0}{2}\rho + \frac{1}{2(2\pi)^n\rho}\int_{\mathbb{R}^n} p^2\left[\left(1+\frac{2\rho\hat{V}_p}{p^2}\right)^{1/2} - 1 - \frac{\rho\hat{V}_p}{p^2}\right]dp \\ &= \frac{1}{2}\left\{\hat{V}_0 - \frac{1}{2(2\pi)^n}\int \frac{\hat{V}_p^2}{p^2}\,dp\right\}\rho + Q(\rho), \end{aligned} \tag{2.1.2}$$

where

$$Q(\rho) := \frac{1}{2(2\pi)^n\rho}\int_{\mathbb{R}^n} p^2\left[\left(1+\frac{2\rho\hat{V}_p}{p^2}\right)^{1/2} - 1 - \frac{\rho\hat{V}_p}{p^2} + \frac{\rho^2\hat{V}_p^2}{2p^4}\right]dp.$$

We recognize the terms in the curly brackets in (2.1.2) as the the first two terms in the Born series (Section 1.2), which we denote by $8\pi a_0$ respectively $8\pi a_1$. Assume that $n = 3$. By a change of variables $p \mapsto (\hat{V}_0\rho)^{1/2}p$ and the dominated convergence theorem, we find that

$$\lim_{\rho\to 0}\frac{Q(\rho)}{\rho^{3/2}\hat{V}_0^{5/2}} = \frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3} p^2\left[\left(1+\frac{2}{p^2}\right)^{1/2} - 1 - \frac{1}{p^2} + \frac{1}{2p^4}\right]dp = \frac{1}{2(8\pi)^{3/2}}\frac{128}{15\sqrt{\pi}},$$

and hence

$$Q(\rho) = 4\pi a_0\rho\frac{128}{15\sqrt{\pi}}\left(a_0^3\rho\right)^{1/2} + o\left(\rho^{3/2}\right) \quad \text{as } \rho\to 0.$$

Thus we have shown the asymptotic formula

$$e_0^{\mathrm{Bog}}(\rho) = 4\pi(a_0+a_1)\rho + 4\pi a_0\rho\frac{128}{15\sqrt{\pi}}(a_0^3\rho)^{1/2} + o\left(\rho^{3/2}\right) \quad \text{as } \rho\to 0.$$

Assuming that indeed $e_0^{\mathrm{Bog}}(\rho) \approx e_0(\rho)$ and replacing $a_0 + a_1$ respectively a_0 with the full scattering length a, we arrive at the Lee-Huang-Yang Formula. We end this chapter by remarking that, using the CCR, the Bogoliubov ground state above may be written in the form

$$\Psi^{\mathrm{Bog}} = \exp\left(\frac{1}{2}\sum_{p\neq 0} c_p a_p^+ a_{-p}^+ + \sqrt{N_0}a_0^+\right)|0\rangle, \tag{2.1.3}$$

where

$$c_p := \frac{1-\sqrt{1+2\rho p^{-2}\hat{V}_p}}{1-\sqrt{1+2\rho p^{-2}\hat{V}_p}}.$$

In Section 3.3 we shall use the ansatz in (2.1.3), not a priori fixing the c_p's.

Chapter 3

The Ground State Energy in Dimension $n > 3$

Abstract: We consider a Bose gas in spatial dimension $n > 3$ with a repulsive, radially symmetric two-body potential V. In the limit of low density ρ, the ground state energy per particle in the thermodynamic limit is shown to be $(n-2)|\mathbb{S}^{n-1}|a^{n-2}\rho$, where $|\mathbb{S}^{n-1}|$ denotes the surface measure of the unit sphere in $\mathbb{R}^n$ and a is the scattering length of V. Furthermore, for smooth and compactly supported two-body potentials, we derive upper bounds to the ground state energy with a correction term $(1+\gamma)8\pi^4 a^6\rho^2|\ln(a^4\rho)|$ in dimension $n = 4$, where $0 < \gamma \leq C\|V\|_\infty^{1/2}\|V\|_1^{1/2}$, and a correction term which is $\mathcal{O}(\rho^2)$ in higher dimensions.

3.1 Introduction

The experimental realization of Bose-Einstein Condensation in 1995 [1] has inspired renewed interest in a rigorous understanding of the interacting Bose gas, and in particular the ground state energy. The typical model for the energy of N bosons enclosed in a box $\Lambda = \Lambda_L := (-L/2, L/2)^n$, is the Hamiltonian

$$H_{N,L} = \sum_{i=1}^{N} -\Delta_i + \sum_{1\leq j<k\leq N} V(x_j - x_k) \tag{3.1.1}$$

on $L^2_{\text{sym}}(\Lambda^N)$ (the set of totally symmetric L^2-functions on Λ^N). Here units are chosen such that $\hbar^2/2m = 1$, where m is the mass of a particle. We will always assume that the two-body potential V is a nonnegative and radially symmetric function on $\mathbb{R}^n$. Let

$$E_0(N, L) := \inf \sigma(H_{N,L}) = \inf\{\langle\Psi, H_{N,L}\Psi\rangle : \|\Psi\| = 1\}$$

denote the ground state energy of the Bose gas, and let

$$e_0(\rho) := \lim_{N\to\infty} \frac{E_0(N, (N/\rho)^{1/n})}{N} \tag{3.1.2}$$

denote the ground state energy per particle in the thermodynamic limit at density $\rho > 0$. The latter is independent of whatever boundary conditions imposed on Λ. We let a denote the scattering length of V (see section 3.2) and note that $Y := a^n\rho$ is a dimensionless quantity.

In dimension $n = 3$, the asymptotic behavior of $e_0(\rho)$ in the limit of low density was studied by Bogoliubov [2], Lee-Yang [10] and Lee-Huang-Yang [9] in the 1940-50's. In particular, the latter applied the pseudopotential method to derive the expansion

$$e_0(\rho) = 4\pi a\rho\left(1 + \frac{128}{15\sqrt{\pi}}Y^{1/2} + o\big(Y^{1/2}\big)\right) \quad \text{as } Y \to 0,$$

now known as the Lee-Huang-Yang formula (LHY). To give a mathematical proof of LHY is still an open problem, except in a special case of ρ in a so-called simultaneously weak coupling and high density regime, and for a rather narrow class of potentials [6]. Even to prove the leading order term in LHY turned out to be a hard problem: A variational calculation carried out by Dyson in 1957 [3] showed the upper bound $e_0(\rho) \le 4\pi a\rho(1 + CY^{1/3})$, for hard-core interactions. This has later been generalized to general nonnegative, radially symmetric potentials [13]. However, no proof of a matching, leading order lower bound was available until 1998, where Lieb-Yngvason managed to show that $e_0(\rho) \ge 4\pi a\rho(1 - CY^{1/17})$. Their approach was improved in [8] to yield $e_0(\rho) \ge 4\pi a\rho(1 - C\rho^{1/3}|\ln\rho|^3)$. At the present time, no lower bound has captured even the correct order in the expansion parameter Y in LHY. For the upper bound there has been success though: In [4] a trial state of the form

$$\Psi = \exp\left(\frac{1}{2}\sum_{p\neq 0} c_p a_p^+ a_{-p}^+ + \sqrt{N_0}a_0^+\right)|0\rangle \tag{3.1.3}$$

was used to derive an upper bound

$$e_0(\rho) \le 4\pi a\rho\left(1 + \frac{128}{15\sqrt{\pi}}(1 + C\lambda)Y^{1/2}\right) + \tilde{C}\rho^2|\ln\rho|,$$

for a coupled two-body potential $V = \lambda\tilde{V}$. While the correction term has the correct order in Y, the constant is only correct in the limit of weak coupling, $\lambda \to 0$. The (Fock) trial state (3.1.3) is inspired by the Bogoliubov approximation, and the crucial feature is that particles of nonzero momenta appear only in *pairs* of opposite momenta. Similar states have previously been considered by Girardeau-Arnowitt [5] and Solovej [22] in the context of Bose gases. In a paper from 2009 [25] Yau-Yin introduced a new trial state, extending the properties of (3.1.3). More precisely, they include pairs with total momentum of order $\rho^{1/2}$ (however their trial state has a fixed number of particles in contrast to (3.1.3)). This turns out to lower the energy significantly and their result is an upper bound consistent with LHY. We note however that the calculation with the Yau-Yin trial state is somewhat more involved than the computation with (3.1.3).

The model (3.1.1) has also been studied in other dimensions. The case $n = 1$ (with a delta-function potential) was already considered back in 1963 by Lieb-Liniger [12] and turned out to be exactly solvable. In two dimensions, the leading order term was, to our knowledge, first identified by Schick [20] in 1971 to be $4\pi\rho|\ln(a^2\rho)|^{-1}$. This was rigorously proven to be correct by Lieb-Yngvason in 2001 [15]. To our knowledge there are yet no rigorous results on the 2-dimensional correction term (in fact, it seems that there is not even consensus about what this term should be: compare e.g. [20], [24] and [17]). In [24] Yang reexamined the pseudopotential method in dimension two, four and five. In the latter he found the method inconclusive, while he in four dimensions derived the expansion

$$e_0(\rho) = 4\pi^2 a^2 \rho\big[1 + 2\pi^2 Y|\ln Y| + o\big(Y \ln Y\big)\big] \quad \text{as } Y \to 0. \tag{3.1.4}$$

We remark that in Yangs paper the correction $2\pi^2 Y|\ln Y|$ appears to be $4\pi^2 Y|\ln Y|$, due to a minor miscalculation.

In this paper we test some of the rigorous 3-dimensional calculations in higher dimensions. We follow the proofs of Dyson and Lieb-Yngvason to obtain the n-dimensional upper- and lower bounds (Theorem 3.2.2 and Theorem 3.2.3),

$$1 - CY^{\alpha} \le \frac{e_0(\rho)}{s_n a^{n-2}\rho} \le 1 + CY^{\beta}, \tag{3.1.5}$$

where $s_n := (n-2)|\mathbb{S}^{n-1}|$, $|\mathbb{S}^{n-1}|$ denotes the surface measure of the unit sphere in $\mathbb{R}^n$ and where

$$\alpha = \frac{n-2}{n(n+2)+2} \quad \text{and} \quad \beta = \frac{n-2}{n}.$$

Secondly, we employ the trial state (3.1.3) to improve the upper bounds. In dimension $n = 4$ we show that (Theorem 3.3.1)

$$e_0(\rho) \le 4\pi^2 a^2 \rho\big[1 + 2\pi^2(1+\gamma)Y|\ln Y|\big] + C_V \rho^2,$$

where $0 < \gamma \le C\|V\|_\infty^{1/2}\|V\|_1^{1/2}$, consistent with (3.1.4) in the limit of weak coupling. In dimension $n \ge 5$ the calculation yields the upper bound (Theorem 3.3.1)

$$e_0(\rho) \le s_n a^{n-2}\rho + C\rho^2.$$

The second order asymptotics of $e_0(\rho)$ becomes more subtle in dimension $n > 3$. The correction to the energy is given in terms of certain integrals, which, in three dimensions, are exactly computable in the limit $\rho \to 0$, in a straight-forward manner. This is not the case in higher dimensions, and a more careful analysis has to be carried out. In dimension $n \ge 5$ we have not been able to identify the expansion parameter Y in the correction term, nor an explicit coefficient.

Finally, since (3.1.3) is a Fock state, we need the fact that the canonical ground state energy defined in (3.1.2) can be recovered from the grand-canonical setting. Although this is a well-known result, we did not come across a good reference for it, and hence we have included a proof in Appendix 3.A.

3.2 The Leading Order Term

In this section we prove the upper and lower bounds in (3.1.5). We will assume that V is a nonnegative, radial and measurable function on $\mathbb{R}^n$, where $n \ge 3$. The scattering length of V is denoted by a and may be defined via the variational problem (see e.g. [11], [26])

$$s_n a^{n-2} := \inf_u \int_{\mathbb{R}^n} |\nabla u|^2 + \frac{1}{2} V u^2, \tag{3.2.1}$$

where the infimum is taken over all nonnegative, radially symmetric functions $u \in H^1_{\text{loc}}(\mathbb{R}^n)$ satisfying $u(r) \to 1$ as $r \to \infty$. Notice that such functions are automatically continuous away from the origin. Also, it is easy to see that we may restrict attention to radially increasing functions. Moreover, we remark that a is finite if and only if V is integrable at infinity. In many cases the infimum in (3.2.1) is a unique minimum, and the minimizer u satisfies the zero-energy scattering equation

$$-\Delta u + \frac{1}{2} V u = 0 \tag{3.2.2}$$

in the sense of distributions on $\mathbb{R}^n$. The existence of a scattering solution for a nonnegative, radially symmetric and *compactly supported* potential is established in [15]. We note briefly some properties of the scattering solution u, referring to [15], [11] for details:

(i) For large r, $u(r) \approx 1 - (a/r)^{n-2}$, or more precisely

$$\lim_{r\to\infty} \frac{1-u(r)}{(a/r)^{n-2}} = 1. \tag{3.2.3}$$

In fact

$$u(r) \geq 1 - (a/r)^{n-2}, \tag{3.2.4}$$

with equality for $r > R_0$ if $\text{supp}(V) \subset B(0, R_0)$.

(ii) Monotonicity: If $V \leq \tilde{V}$, then $a \leq \tilde{a}$, while $u \geq \tilde{u}$.

(iii) Regularity imposed on V is inherited by u. For instance, one may apply elliptic regularity and Sobolev imbedding's to show that if V is smooth, so is u.

(iv) For $V \in L^1(\mathbb{R}^n)$, it follows from (4.B.2) that u can be represented as

$$1 - u(x) = \frac{1}{2}\Gamma(Vu)(x) := \frac{1}{2s_n} \int_{\mathbb{R}^n} \frac{V(y)u(y)}{|x-y|^{n-2}}\, dy. \tag{3.2.5}$$

By (3.2.3) and the dominated convergence theorem it then follows that

$$2s_n a^{n-2} = \int_{\mathbb{R}^n} V(x)u(x)\, dx. \tag{3.2.6}$$

The main result of this section is the following, which is an immediate consequence of Theorem 3.2.2 and Corollary 3.2.10 below.

Theorem 3.2.1. *Let $n \geq 3$ and suppose that V is nonnegative, radially symmetric, measurable and decays faster than $r^{-\nu}$ at infinity, where $\nu = (6n-2)/5$. Suppose furthermore that V admits a scattering solution. Then*

$$\lim_{\rho\to 0} \frac{e_0(\rho)}{s_n a^{n-2} \rho} = 1. \tag{3.2.7}$$

3.2.1 The Upper Bound

We have the following dimensional generalization of [3], [11].

Theorem 3.2.2. *Let $n \geq 3$ and suppose that V is nonnegative, radially symmetric and measurable.*

(i) Without further assumptions,

$$\limsup_{\rho \to 0} \frac{e_0(\rho)}{s_n a^{n-2} \rho} \leq 1.$$

(ii) There exist $C, \delta > 0$ independent of V such that, if V admits a scattering solution, then

$$e_0(\rho) \leq s_n a^{n-2} \rho \big[1 + C Y^{1-2/n} \big],$$

whenever $Y \leq \delta$.

Proof. We employ the periodic trial state of Dyson [3]. This state is not symmetric, but since the ground state of $H_{N,L}$ on the full space $L^2(\Lambda^N)$ *is* symmetric [11], we obtain an upper bound to $e_0(\rho)$. Suppose that $u \in H^1_{\text{loc}}(\mathbb{R}^n)$ is nonnegative, radially symmetric, increasing and moreover that $u(r) \to 1$ as $r \to \infty$. The trial state is then defined by

$$\Psi := F_2 \cdot F_3 \cdots F_N,$$

where

$$F_i := \min_{1 \leq j < i} \left[\min_{m \in \mathbb{Z}} f(x_i - x_j - mL) \right]$$

and

$$f(r) := \begin{cases} \frac{u(r)}{u(b)} & 0 \leq r \leq b \\ 1 & r > b \end{cases},$$

for some (large) $b > 0$ to be chosen. Following the calculation in [11] we obtain

$$e_0(\rho) \leq \frac{J\rho + \frac{2}{3}(K\rho)^2}{(1 - I\rho)^2}, \tag{3.2.8}$$

where

$$I := \int (1 - f(x)^2)\, dx, \quad K := \int f(x) |\nabla f(x)|\, dx$$

and

$$J := \int |\nabla f(x)|^2 + \frac{1}{2} V(x) f(x)^2\, dx.$$

It follows that

$$\limsup_{\rho \to 0} e_0(\rho)\rho^{-1} \leq J \leq \frac{1}{u(b)^2} \int |\nabla u(x)|^2 + \frac{1}{2} V(x) u(x)^2\, dx,$$

where we have used

$$f(r) \leq \frac{u(r)}{u(b)} \quad \text{and} \quad f'(r) \leq \frac{u'(r)}{u(b)}$$

in the latter inequality. In the limit $b \to \infty$ we get

$$\limsup_{\rho\to 0} e_0(\rho)\rho^{-1} \le \int |\nabla u(x)|^2 + \frac{1}{2}V(x)u(x)^2\, dx,$$

and minimizing over u yields (i), by definition of the scattering length.

In case V admits a scattering solution, we apply the above construction with u being this particular function. The bound (3.2.4) then allow us to estimate more explicitly. Indeed, we have $f(r) \ge [1-(a/r)^{n-2}]_+$, and hence

$$I \le |\mathbb{S}^{n-1}|\left(\int_0^a r^{n-1}\, dr + \int_a^b 2a^{n-2}r\, dr\right) \le |\mathbb{S}^{n-1}|a^{n-2}b^2.$$

Next,

$$J \le \frac{s_n a^{n-2}}{u(b)^2} \le \frac{s_n a^{n-2}}{(1-(a/b)^{n-2})^2},$$

provided $b > a$. Finally, using $f(r) \le 1$ and an integration by parts yields

$$K \le |\mathbb{S}^{n-1}| \int_0^b f'(r)r^{n-1}\, dr \le |\mathbb{S}^{n-1}| \left(b^{n-1} - (n-1)\int_0^b f(r)r^{n-2}\, dr\right).$$

However,

$$\begin{aligned}\int_0^b f(r)r^{n-2}\, dr &\ge \int_a^b \left[1-(a/r)^{n-2}\right]r^{n-2}\, dr \\ &= \frac{b^{n-1}}{n-1} - a^{n-2}b + \frac{n-2}{n-1}a^{n-1} \ge \frac{b^{n-1}}{n-1} - a^{n-2}b,\end{aligned}$$

and hence $K \le |\mathbb{S}^{n-1}|(n-1)a^{n-2}b$. Now, by choosing $b := (|\mathbb{S}^{n-1}|\rho)^{-1/n}$, we have

$$(a/b)^{n-2} = |\mathbb{S}^{n-1}|a^{n-2}b^2\rho = \tilde{Y}^\beta,$$

where $\tilde{Y} := |\mathbb{S}^{n-1}|Y$ and $\beta := (n-2)/n$. In total we have

$$e_0(\rho) \le s_n a^{n-2}\rho\left[\frac{1}{(1-\tilde{Y}^\beta)^4} + \frac{CY^\beta}{(1-\tilde{Y}^\beta)^2}\right] \le s_n a^{n-2}\rho\big(1+\tilde{C}Y^\beta\big),$$

provided $\tilde{Y}$ is bounded away from 1. □

3.2.2 The Lower Bound

In this section we prove an n-dimensional lower bound by following the steps in [14]. The assumption of compact support in Theorem 3.2.3 below is relaxed in Corollary 3.2.10.

Theorem 3.2.3. *Let $n \ge 3$ and suppose that V is nonnegative, radially symmetric, measurable and compactly supported with, say, supp$(V) \subset B(0, R_0)$. There exist $C, \delta > 0$ independent of V such that*

$$e_0(\rho) \ge s_n a^{n-2}\rho\big(1 - CY^\alpha\big),$$

where

$$\alpha := \frac{n-2}{n(n+2)+2}, \tag{3.2.9}$$

provided

$$Y \leq \min\left\{\delta, (a/R_0)^{\frac{n-2}{5\alpha}}\right\}. \tag{3.2.10}$$

In order to prove Theorem 3.2.3 we consider $H = H_{N,L}$ with Neumann boundary conditions on Λ. The first step is to obtain an n - dimensional version of Dyson's lemma. In what follows we set

$$a_n := (n-2)a^{n-2}.$$

Lemma 3.2.4 (Dyson's Lemma)**.** *Suppose that U is a measurable, nonnegative and radially symmetric function on $\mathbb{R}^n$, which satisfies*

$$U(r) = 0, \quad \text{for } r \leq R_0, \quad \text{and} \quad \int_0^\infty U(r) r^{n-1}\, dr \leq 1.$$

Let $B \subseteq \mathbb{R}^n$ be open and star shaped w.r.t. the origin. Then

$$\int_B |\nabla\varphi(x)|^2 + \frac{1}{2}V(x)|\varphi(x)|^2\, dx \geq a_n \int_B U(x)|\varphi(x)|^2\, dx,$$

for each $\varphi \in H^1(B)$.

Proof. For any $\omega \in \mathbb{S}^{n-1}$ we let

$$R(\omega) = \sup\{r \geq 0 : s\omega \in B, \text{ for each } 0 \leq s \leq r\}$$

denote the (possibly infinite) distance from the origin to the boundary of B in the direction of ω. Since B is open and star shaped w.r.t. the origin, it follows that, for any $r \geq 0$, $r\omega \in B$ if and only if $r < R(\omega)$. By passing into polar coordinates, we then see that it suffices to show that, for each fixed $\omega \in \mathbb{S}^{n-1}$,

$$\int_0^{R(\omega)} \big(|f'(r)|^2 + \frac{1}{2}V(r)|f(r)|^2\big) r^{n-1}\, dr \geq a_n \int_0^{R(\omega)} U(r)|f(r)|^2 r^{n-1}\, dr, \tag{3.2.11}$$

where $f(r) := \varphi(r\omega)$ with $|f'(r)| \leq |\nabla\varphi(r\omega)|$. We may assume that $R(\omega) > R_0$, since otherwise the right hand side in (3.2.11) vanishes, and we claim that

$$\int_0^{R(\omega)} \big(|f'(r)|^2 + \frac{1}{2}V(r)|f(r)|^2\big) r^{n-1}\, dr \geq a_n |f(R)|^2, \tag{3.2.12}$$

for each $R_0 < R < R(\omega)$. Indeed, if $f(R) \neq 0$, then the function u given by $u(x) = |f(|x|)/f(R)|$ for $|x| \leq R$ and $u(x) = 1$ for $|x| > R$ is admissible in (3.2.1), and since $V(r) = 0$, for $r > R$, it follows that

$$s_n a^{n-2} \leq \frac{|\mathbb{S}^{n-1}|}{|f(R)|^2} \int_0^{R(\omega)} \big(|f'(r)|^2 + \frac{1}{2}V(r)|f(r)|^2\big) r^{n-1}\, dr.$$

Now (3.2.11) follows by multiplying both sides of (3.2.12) with $U(R)R^{n-1}$ and then integrating w.r.t. R. □

Corollary 3.2.5. *Suppose that U satisfies the conditions of Lemma 3.2.4, and define*

$$W := \sum_{i=1}^{N} U \circ t_i, \quad t_i(x_1, \dots, x_N) := \min_{j \neq i} |x_i - x_j|.$$

Then $H \geq a_n W$.

Proof. Since V is nonnegative and radial,

$$\sum_{i=1}^{N} V(t_i(\vec{x})) \leq \sum_{i=1}^{N} \sum_{j<i} V(x_i - x_j) + \sum_{i=1}^{N} \sum_{j>i} V(x_i - x_j) = 2 \sum_{i<j} V(x_i - x_j),$$

for each $\vec{x} = (x_1, \dots, x_N)$, and hence

$$H \geq \sum_{i=1}^{N} \big(-\Delta_i + \frac{1}{2} V \circ t_i \big). \tag{3.2.13}$$

We focus on the first term $i = 1$, and fix $x_2, \dots, x_N \in \Lambda$. For $j \neq 1$ define

$$B_j = \{x_1 \in \Lambda : t_1(\vec{x}) = |x_1 - x_j|\}.$$

Fix an arbitrary $\psi \in H^1(\Lambda^N)$. By a change of variables $x_1 \mapsto x_1 + x_j$, and by noting that $(B_j - x_j)$ is star shaped w.r.t. the origin (indeed convex), we may apply Dyson's lemma to obtain

$$\int_{B_j} |\nabla_1 \psi(\vec{x})|^2 + \frac{1}{2} V(t_i(\vec{x})) |\psi(\vec{x})|^2 \, dx_1 \geq a_n \int_{B_j} U(t_1(\vec{x})) |\psi(\vec{x})|^2 \, dx_1, \tag{3.2.14}$$

for each $j \neq 1$. Moreover, since the B_j's cover Λ disjointly (a.e.), we conclude that (3.2.14) holds with B_j replaced by Λ. Then, by Fubini's theorem,

$$\int_{\Lambda^N} |\nabla_1 \psi(\vec{x})|^2 + \frac{1}{2} V(t_1(\vec{x})) |\psi(\vec{x})|^2 \, d\vec{x} \geq a_n \int_{\Lambda^N} U(t_1(\vec{x})) |\psi(\vec{x})|^2 \, d\vec{x}.$$

We get analogous contributions from $i = 2, \dots, N$ in (3.2.13), and upon adding them, we obtain the result. □

We now combine Corollary 3.2.5 with Temple's inequality [18] in a perturbative approach. The parameters R and ε appearing below will be chosen appropriately later on.

Lemma 3.2.6. *Let $0 < \varepsilon < 1$ and $R_0 < R < L/2$. Suppose that*

$$G(N, L) := \varepsilon \pi^2 L^{-2} - s_n a^{n-2} L^{-n} N^2 > 0.$$

Then

$$E_0(N, L) \geq N(N-1) K(N, L),$$

where

$$K(N, L) := \frac{s_n a^{n-2}}{L^n} (1 - \varepsilon) \left(1 - \frac{2R}{L} \right)^n \left(1 - v_n \frac{R^n}{L^n} \right)^{N-2} \left(1 - \frac{n(n-2) a^{n-2} N}{(R^n - R_0^n) G(N, L)} \right)$$

Here v_n denotes the measure of the unit ball in $\mathbb{R}^n$.

Proof. Suppose that U and W are as in Lemma 3.2.4 respectively Corollary 3.2.5. Together with the fact that V is nonnegative, we then have a lower bound

$$H = \varepsilon H + (1-\varepsilon)H \geq -\varepsilon\Delta + (1-\varepsilon)a_n W =: \tilde{H},$$

and consequently

$$E_0(N,L) \geq \tilde{E}_0(N,L) := \inf \sigma(\tilde{H}). \tag{3.2.15}$$

We estimate $\tilde{E}_0(N,L)$ by employing Temple's inequality in the ground state of $-\varepsilon\Delta$ (with Neumann Boundary conditions), which is the constant function $\varphi_0(x) \equiv |\Lambda|^{-N/2}$ with corresponding eigenvalue zero. Given any operator A on $L^2(\Lambda^N)$ with domain containing φ_0, we let $\langle A\rangle = \langle \varphi_0, A\varphi_0\rangle$. Temple's inequality and (3.2.15) yields

$$\begin{aligned} E_0(N,L) &\geq \langle \tilde{H}\rangle - \frac{\langle \tilde{H}^2\rangle - \langle \tilde{H}\rangle^2}{\tilde{E}_1 - \langle \tilde{H}\rangle} \\ &= (1-\varepsilon)a_n\langle W\rangle - \frac{(1-\varepsilon)^2 a_n^2\big(\langle W^2\rangle - \langle W\rangle^2\big)}{\tilde{E}_1 - (1-\varepsilon)a_n\langle W\rangle}, \end{aligned}$$

provided $\langle \tilde{H}\rangle < \tilde{E}_1$, where $\tilde{E}_1$ is the second lowest eigenvalue of $\tilde{H}$. Note however that, since W is nonnegative, we have $\tilde{H} \geq -\varepsilon\Delta$, and hence $\tilde{E}_1 \geq \varepsilon\pi^2/L^2$, which is the second lowest eigenvalue of $-\varepsilon\Delta$. We now choose the function U to be

$$U(r) := \begin{cases} n(R^n - R_0^n)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise} \end{cases}.$$

By discarding the term $\langle W\rangle^2$, replacing $(1-\varepsilon)$ by 1 in two appropriate places and employing the fact that

$$\langle W^2\rangle \leq n\cdot N(R^n - R_0^n)^{-1}\langle W\rangle,$$

we obtain

$$E_0(N,L) \geq (1-\varepsilon)a_n\langle W\rangle\left[1 - \frac{n a_n N}{(R^n - R_0^n)\big(\varepsilon\pi^2/L^2 - a_n\langle W\rangle\big)}\right], \tag{3.2.16}$$

provided $a_n\langle W\rangle < \varepsilon\pi^2/L^2$. To estimate this further, we need upper and lower bounds on $\langle W\rangle$, and we claim that

$$\frac{|\mathbb{S}^{n-1}|}{L^n}N(N-1)\big(1-2R/L\big)^n\big(1 - v_n R^n/L^n\big)^{N-2} \leq \langle W\rangle \leq \frac{|\mathbb{S}^{n-1}|}{L^n}N(N-1). \tag{3.2.17}$$

This will conclude the proof of the lemma. For the upper bound in (3.2.17) we fix $x_1 \in \Lambda$ and notice that

$$\big\{(x_2,\ldots,x_N) \in \Lambda^{N-1} : R_0 < t_1(\vec{x}) < R\big\} \subseteq \bigcup_{j=2}^{N} F_j,$$

where $\vec{x} = (x_1, \ldots, x_N)$ and $F_j = \Lambda^{N-1}$, except that the j'th factor is replaced by $B(x_1, R)\backslash B(x_1, R_0)$. It follows that

$$\int_{\Lambda^{N-1}} U(t_1(\vec{x}))\, dx_2 \ldots dx_N \leq \frac{n}{R^n - R_0^n} \sum_{j=2}^{N} |F_j| = |\mathbb{S}^{n-1}|(N-1)|\Lambda|^{N-2}.$$

By integrating over $x_1 \in \Lambda$ and then adding the identical contributions from the integrals of $U(t_2), \ldots, U(t_N)$, we arrive at the upper bound in (3.2.17). To verify the lower bound, we let $\Lambda' \subseteq \Lambda$ denote the cube with same center as Λ but with side length $L - 2R$. Fix $x_1 \in \Lambda'$ and notice that $B(x_1, R) \subseteq \Lambda$. We then have

$$\bigcup_{j=2}^{N} E_j \subseteq \big\{(x_2, \ldots, x_N) \in \Lambda^{N-1} : R_0 < t_1(\vec{x}) < R\big\}, \tag{3.2.18}$$

where

$$E_j = (\Lambda\backslash B(x_1, R))^{N-1}$$

except again that the j'th factor is replaced by $B(x_1, R)\backslash B(x_1, R_0)$. Since the E_j's are pairwise disjoint, (3.2.18) implies that

$$\int_{\Lambda^{N-1}} U(t_1(\vec{x}))\, dx_2 \ldots dx_N \geq \frac{n}{R^n - R_0^n} \sum_{j=2}^{N} |E_j| = |\mathbb{S}^{n-1}|(N-1)(|\Lambda| - v_n R^n)^{N-2},$$

and integrating over $\Lambda \supset \Lambda' \ni x_1$, we obtain

$$\int_{\Lambda^N} U(t_1(\vec{x}))\, d\vec{x} \geq |\mathbb{S}^{n-1}|(N-1)(L-2R)^n(|\Lambda| - v_n R^n)^{N-2}.$$

Again, by adding identical contributions from the integrals of $U(t_2), \ldots, U(t_N)$, we have proved (3.2.17) and with it the lemma. □

Note that, for fixed $\rho > 0$,

$$G(\rho L^n, L) \leq \pi^2 L^{-2} - s_n a^{n-2} \rho^2 L^n < 0,$$

for large L, so Lemma 3.2.6 may not immediately be applied to get estimates in the thermodynamic limit.

Lemma 3.2.7. *The mapping $N \mapsto E_0(N, L)$ is superadditive, i.e.,*

$$E_0(k+m, L) \geq E_0(k, L) + E_0(m, L), \quad \textit{for all } k, m \in \mathbb{N}.$$

Proof. Fix an arbitrary normalized $\psi \in H^1(\Lambda^{k+m})$. Since V is nonnegative, it follows that

$$\begin{aligned} \langle \psi, H\psi \rangle \quad &\geq \quad \int_{\Lambda^{k+m}} \sum_{i=1}^{k} |\nabla_i \psi|^2 + \sum_{1 \leq i < j \leq k} V(x_i - x_j)|\psi|^2 \\ &+ \quad \int_{\Lambda^{k+m}} \sum_{i=k+1}^{k+m} |\nabla_i \psi|^2 + \sum_{k+1 \leq i < j \leq k+m} V(x_i - x_j)|\psi|^2. \end{aligned} \tag{3.2.19}$$

Then, by Fubini's theorem,

$$\int_{\Lambda^{k+m}} \sum_{i=1}^{k} |\nabla_i \psi|^2 + \sum_{1\le i<j\le k} V(x_i - x_j)|\psi|^2 \ge \int_{\Lambda^m} \left(E_0(k,L) \int_{\Lambda^k} |\psi|^2 \right) = E_0(k,L),$$

and similarly for the second term on the right-hand side in (3.2.19) . □

Lemma 3.2.8. *Suppose that $L/l \in \mathbb{N}$. Then*

$$E_0(N,L) \ge M \cdot \min \sum_{m=0}^{N} c_m E_0(m,l), \tag{3.2.20}$$

where $M := (L/l)^n$ and where the minimum is over all tuples $(c_0, \ldots, c_N)$ of numbers $c_m \ge 0$ subject to the conditions

$$\sum_{m=0}^{N} c_m = 1 \quad \text{and} \quad \sum_{m=0}^{N} m c_m = N/M. \tag{3.2.21}$$

Proof. We partition Λ into M disjoint boxes $\Lambda_1, \ldots, \Lambda_M$, each of side length l. Correspondingly we have a partition $\{\Omega_\beta\}$ of Λ^N,

$$\Omega_\beta := \Lambda_{\beta_1} \times \ldots \times \Lambda_{\beta_N}, \quad \beta = (\beta_1, \ldots, \beta_N),\ 1 \le \beta_j \le M,$$

and hence

$$\langle \psi, H\psi \rangle = \sum_\beta \int_{\Omega_\beta} \sum_{i=1}^{N} |\nabla_i \psi|^2 + \sum_{i<j} V(x_i - x_j)|\psi|^2. \tag{3.2.22}$$

Fix a β as above. By Fubini's theorem, the integration regime Ω_β may be replaced by $\Lambda_1^{\alpha_1} \times \ldots \times \Lambda_M^{\alpha_M}$, for some multiindex $\alpha \in \mathbb{N}_0^M$ with length $|\alpha| = N$. For each $0 \le m \le N$, we let $M \cdot c_m$ denote the number of components of α equal to m. By following the proof of Lemma 3.2.7, we split the kinetic energy into appropriate terms, and discard interactions between particles in different boxes to obtain the lower bound

$$\begin{aligned} \int_{\Omega_\beta} \cdots \quad &\ge \quad \left(\int_{\Omega_\beta} |\psi|^2 \right) \sum_{j=1}^{M} E_0(\alpha_j, l) \\ &= \quad \left(\int_{\Omega_\beta} |\psi|^2 \right) M \sum_{m=0}^{N} c_m E_0(m,l) \\ &\ge \quad \left(\int_{\Omega_\beta} |\psi|^2 \right) M \min \left(\sum_{m=0}^{N} c_m E_0(m,l) \right). \end{aligned}$$

Employing this estimate in (3.2.22) yields the result. □

Lemma 3.2.9. *Let $\rho = N/L^n$. Suppose that $L/l \in \mathbb{N}$, $R_0 < R < l/2$ and $G(4\rho l^n, l) > 0$. Then*

$$\frac{E_0(N,L)}{N} \ge (\rho l^n - 1) K(4\rho l^n, l).$$

Proof. Suppose that $c_m \geq 0$ satisfies (3.2.21). We split the sum in (3.2.20) into two parts:

$$\sum_m c_m E_0(m,l) = \sum_{m<p} c_m E_0(m,l) + \sum_{m\geq p} c_m E_0(m,l), \tag{3.2.23}$$

for some $p \in \mathbb{N}$ to be chosen. Suppose for now that $G(p,l) > 0$. Since $G(N,L)$ and $K(N,L)$ are decreasing functions of N, Lemma 3.2.6 implies that

$$E_0(m,l) \geq m(m-1)K(p,l), \quad \text{for } 0 \leq m \leq p, \tag{3.2.24}$$

and hence

$$\sum_{m<p} c_m E_0(m,l) \geq K(p,l) \sum_{m<p} c_m m(m-1).$$

Let $t := \sum_{m<p} mc_m$. By the Cauchy-Schwarz inequality,

$$t^2 \leq \left(\sum_{m<p} m^2 c_m\right)\left(\sum_{m<p} c_m\right) \leq \sum_{m<p} m^2 c_m,$$

and it follows that

$$\sum_{m<p} c_m m(m-1) \geq t(t-1).$$

Thus we have

$$\sum_{m<p} c_m E_0(m,l) \geq K(p,l)t(t-1).$$

We now employ the superadditivity of $m \mapsto E_0(m,l)$ (Lemma 3.2.7) to obtain a lower bound on the second sum on the right hand side in (3.2.23). For $m \geq p$ we write $m = \lfloor m/p \rfloor p + r$, where $\lfloor m/p \rfloor$ denotes the lower integer part of m/p and $r \in \mathbb{N}_0$ is the remainder. Notice that $\lfloor m/p \rfloor \geq m/(2p)$ always. The superadditivity of $E_0(m,l)$ then yields

$$E_0(m,l) \geq m/(2p)E_0(p,l),$$

and it follows that

$$\sum_{m\geq p} c_m E_0(m,l) \geq \frac{E_0(p,l)}{2p}(k-t) \geq \frac{1}{2}(p-1)(k-t)K(p,l),$$

where $k := N/M = \rho l^n$. Altogether we have

$$\sum_{m=0}^{N} c_m E_0(m,l) \geq K(p,l)\big[t(t-1) + \frac{1}{2}(p-1)(k-t)\big].$$

The choice $p = \lfloor 4k \rfloor$ implies that $x \mapsto \big(x(x-1) + \frac{1}{2}(p-1)(k-x)\big)$ is decreasing on $[0,k]$, which is where t lies, and hence the minimum is taken at $x = k$. Thus we have that

$$\frac{E_0(N,L)}{N} \geq \frac{1}{\rho l^n} \sum_m c_m E_0(m,l) \geq K(p,l)(k-1),$$

as claimed. $\square$

We can now finish the proof of Theorem 3.2.3.

Proof of Theorem 3.2.3. Suppose that the conditions of Lemma 3.2.9 are satisfied. Recall that $Y = a^n\rho$. Then

$$\begin{aligned}\frac{E_0(N,L)}{N} &\geq s_n a^{n-2}\rho\big(1-\varepsilon\big)\big(1-2nR/l\big)\Big[1-Y^{-1}(a/l)^n\Big]\\ &\times \Big[1-4v_nY(l/a)^n(R/l)^n\Big]\Big[1-\frac{4n(n-2)l^nY}{(R^n-R_0^n)(\varepsilon\pi^2(a/l)^2-16s_nY^2(l/a)^n)}\Big].\end{aligned}$$

We now make the ansatz

$$\varepsilon = Y^\alpha, \quad a/l = Y^\beta, \quad \frac{R^n-R_0^n}{l^n} = Y^\gamma,$$

for exponents $\alpha,\beta,\gamma>0$. In particular this implies that

$$\left(\frac{R}{l}\right)^n = Y^\gamma + \left(\frac{R_0}{a}\right)^n Y^{n\beta} \leq 2Y^\gamma,$$

provided

$$Y \leq \left(\frac{a}{R_0}\right)^{n/(n\beta-\gamma)}. \tag{3.2.25}$$

Thus we have

$$\begin{aligned}\frac{E_0(N,L)}{N} &\geq s_n a^{n-2}\rho\big(1-Y^\alpha\big)\big(1-C_1Y^{\gamma/n}\big)\big(1-Y^{n\beta-1}\big)\big(1-C_2Y^{1+\gamma-n\beta}\big)\\ &\times \left(1-\frac{C_3Y^{1-\alpha-2\beta-\gamma}}{1-C_4Y^{2-\alpha-(n+2)\beta}}\right).\end{aligned}$$

In attempt to fit exponents we choose β and γ such that

$$\gamma/n = \alpha = n\beta - 1,$$

which in particular implies that $1+\gamma-n\beta = 2\alpha$. Now, the optimal choice of α, such that

$$1-\alpha-2\beta-\gamma \geq \alpha \quad \text{and} \quad 2-\alpha-(n+2)\beta > 0,$$

is given in (3.2.9). With this choice the requirements of Lemma 3.2.9 are indeed satisfied if Y is sufficiently small (depending only on the dimension) and if we take $L = kl$, for an integer $k\in\mathbb{N}$. Also (3.2.25) is exactly the latter condition in (3.2.10). By letting $k\to\infty$ we therefore conclude the proof. □

Corollary 3.2.10. *Suppose that V is nonnegative, radial and measurable with a decay $V(r) \leq Cr^{-\nu}$, for large r, where $\nu > (6n-2)/5$. Suppose furthermore that V admits a scattering solution. There exist a constant $C>0$ depending only on n and a $\delta>0$ depending on n, V such that*

$$e_0(\rho) \geq s_n a^{n-2}\rho\big(1-CY^\alpha\big),$$

provided $Y\leq\delta$.

Proof. Let $R > 0$ and define $V_R = V\chi_{B(0,R)}$ with scattering length $a_R \le a$. Since V is nonnegative, replacing V with V_R cannot increase the energy. By Theorem 3.2.3 we then have

$$e_0(\rho) \ge s_n a_R^{n-2}\rho\big(1 - CY_R^\alpha\big) \ge s_n a_R^{n-2}\rho\big(1 - CY^\alpha\big),$$

provided $Y_R := a_R^n\rho$ is sufficiently small and

$$Y_R \le \left(\frac{a_R}{R}\right)^{\frac{n-2}{5\alpha}}. \tag{3.2.26}$$

Denote the scattering solutions of V and V_R by u respectively u_R. Then, by (3.2.6),

$$\begin{aligned} a^{n-2} - a_R^{n-2} &= \frac{1}{2s_n}\int V(x)u(x) - V_R(x)u_R(x)\,dx \\ &\le \frac{1}{2s_n}\int V(x) - V_R(x)\,dx = \frac{1}{2s_n}\int_{|x|\ge R} V(x)\,dx, \end{aligned}$$

where the inequality follows from the fact that $u \le u_R \le 1$. From the decay of V we obtain

$$a_R^{n-2} \ge a^{n-2}\left(1 - \frac{K}{2(n-2)a^{n-2}R^\varepsilon}\right),$$

provided R is sufficiently large. By choosing R such that

$$\frac{K}{2(n-2)a^{n-2}R^\varepsilon} = Y^\alpha,$$

it follows that R is large,

$$a_R^{n-2} \ge a^{n-2}\big(1 - Y^\alpha\big),$$

and (3.2.26) is satisfied, if Y is sufficiently small and $\nu > (6n-2)/5$. □

3.3 A Second Order Upper Bound

In this section we derive a second order upper bound to $e_0(\rho)$ by estimating the energy in the state (3.1.3). The calculation is inspired by [4].

Theorem 3.3.1. *Let $n \ge 3$ and suppose that $V \in C_0^\infty(\mathbb{R}^n)$ is nonnegative and radially symmetric with $V(0) > 0$. There exist $\delta, C > 0$ (depending on n, V) such that*

$$e_0(\rho) \le s_n a^{n-2}\rho\big[1 + (1+\gamma)Q_n\big] + C\Omega_n, \tag{3.3.1}$$

provided $\rho \le \delta$, where

$$\begin{aligned} Q_3 &= \frac{128}{15\sqrt{\pi}}Y^{1/2} & \Omega_3 &= \rho^2|\ln\rho| \\ Q_4 &= 2\pi^2 Y|\ln Y| & \Omega_4 &= \rho^2 \\ Q_n &= C\rho & \Omega_n &= \rho^2, \quad n \ge 5 \end{aligned}$$

and $0 < \gamma \le C'\|V\|_\infty^{1-2/n}\|V\|_1^{2/n}$. Here $C' > 0$ depends only on n.

The assumptions on V in Theorem 3.3.1 are presumably not optimal. In the actual grand-canonical calculation below, we only need V and its Fourier transform to decay sufficiently fast at infinity (depending on the dimension), and of course the latter can be met by imposing finite smoothness on V. We use compact support of V and $V(0) > 0$ in Lemma 3.3.2 below, which allows us to relate the canonical- and 'grand canonical' ground state energies. Presumably the assumption of compact support can be relaxed to a sufficiently fast decay.

In order to prove Theorem 3.3.1 we initially consider (3.1.1) with *Dirichlet* boundary conditions. Our calculation below is carried out in the grand canonical ensemble, and hence we consider the second quantization of $H_{N,L}$

$$H_L := \bigoplus_{N=0}^{\infty} H_{N,L} \quad \text{on} \quad \mathcal{F}_L := \bigoplus_{N=0}^{\infty} L^2_{\text{sym}}(\Lambda_L^N), \tag{3.3.2}$$

with the corresponding 'grand canonical ground state energy'

$$E_0^{\text{GC}}(N, L) := \inf\left\{\langle H_L\rangle_\Psi : \|\Psi\|_{\mathcal{F}} = 1,\, \langle \mathcal{N}\rangle_\Psi \geq N\right\}, \tag{3.3.3}$$

where $\mathcal{N} = \mathcal{N}_L$ denotes the number operator on $\mathcal{F}_L$ and $\langle A\rangle_\Psi$ denotes the expectation $\langle \Psi, A\Psi\rangle$ of any operator A with Ψ in its domain. Consider the canonical and grand canonical ground state energy *per volume*,

$$e_L(\rho) := \frac{E_0(\rho L^n, L)}{L^n}, \quad e_L^{\text{GC}}(\rho) := \frac{E_0^{\text{GC}}(\rho L^n, L)}{L^n}. \tag{3.3.4}$$

We will assume that the limit

$$e(\rho) := \lim_{L\to\infty} e_L(\rho) \tag{3.3.5}$$

is a convex function of ρ (see e.g. [19]). The following result, which we prove in appendix 3.A, shows that, in the thermodynamic limit, the canonical and grand canonical energies agree.

Lemma 3.3.2. *Suppose that $V \in L^1(\mathbb{R}^n)$ is nonnegative, radially symmetric and compactly supported. Suppose furthermore that $V \geq \varepsilon \chi_{B(0,2R)}$, for some $\varepsilon, R > 0$. Then*

$$e(\rho) = \lim_{L\to\infty} e_L^{GC}(\rho).$$

By (3.3.3) it is clear that $\rho \mapsto e_L^{\text{GC}}(\rho)$ is increasing, for any fixed L. As a consequence we have the following slightly stronger result.

Corollary 3.3.3. *Suppose that V satisfies the assumptions of Lemma 3.3.2, and suppose that $\rho_L \to \rho$ as $L \to \infty$. Then*

$$e(\rho) = \lim_{L\to\infty} e_L^{GC}(\rho_L)$$

Proof. Fix an arbitrary $\varepsilon > 0$. By assumption $e(\rho)$ is convex and hence continuous. Thus we can choose $\delta > 0$ such that

$$|e(\rho) - e(\rho')| \le \varepsilon,$$

for each $\rho' > 0$ with $|\rho - \rho'| \le \delta$. Then, for L sufficiently large,

$$\begin{aligned} e_L^{\mathrm{GC}}(\rho_L) &\ge e_L^{\mathrm{GC}}(\rho - \delta) \\ &= \left[e_L^{\mathrm{GC}}(\rho - \delta) - e(\rho - \delta)\right] + e(\rho - \delta) \\ &\ge \left[e_L^{\mathrm{GC}}(\rho - \delta) - e(\rho - \delta)\right] + e(\rho) - \varepsilon. \end{aligned}$$

By Lemma 3.3.2 it then follows that

$$\liminf_{L\to\infty} e_L^{\mathrm{GC}}(\rho_L) \ge e(\rho) - \varepsilon.$$

Similarly we can show a consistent upper bound, and since ε was arbitrary, the result follows. □

In Section 3.3.1 we construct a *periodic* trial state with an expected number of particles $\langle \mathcal{N} \rangle = \rho L^n$, not directly leading to an upper bound on $e_0(\rho)$ via Lemma 3.3.2. However, Lemma 3.3.4 below, which is essentially proved in [25], shows that given any periodic state, we can find a Dirichlet state on a slightly larger box, with almost as low energy. We let

$$V_L(x) := \sum_{m\in\mathbb{Z}^n} V(x + mL) = \frac{1}{L^n} \sum_{p\in\Lambda_L^*} \hat{V}_p e^{ip\cdot x}, \quad x \in \mathbb{R}^n$$

denote the L-periodization of V, where $\Lambda_L^* := (2\pi/L)\mathbb{Z}^n$ and

$$\hat{V}_p := \int_{\mathbb{R}^n} e^{-ip\cdot x} V(x)\, dx$$

denotes the Fourier transform of V, which is real-valued and radially symmetric, since V is. Then let

$$\tilde{H}_{N,L} := \sum_{i=1}^{N} -\Delta_i + \sum_{1\le j<k\le N} V_L(x_j - x_k)$$

with *periodic* boundary conditions, and let $\tilde{H}_L$ denote its second quantization. Note that, since V is nonnegative, it is clear that $V \le V_L$, and hence the transition from V to V_L cannot decrease the energy. However, since $V_L \to V$ pointwise as $L \to \infty$, we expect the ground state energy of the two systems to coincide in the thermodynamic limit.

Lemma 3.3.4. *Let $L > 2l > 0$. Then*

$$E_0^{GC}(N, L + 2l) \le \langle \tilde{H}_L \rangle_\Psi + C\frac{N}{lL},$$

for each periodic, normalized $\Psi \in \mathcal{F}_L$ with $\langle \mathcal{N} \rangle_\Psi = N$. Here $C > 0$ depends only on n.

We apply Lemma 3.3.4 with $l := \sqrt{L}/2$ and notice that

$$\frac{E_0^{\mathrm{GC}}(\rho L^n, L+2l)}{\rho L^n} = \frac{E_0^{\mathrm{GC}}(\rho_{L+2l}(L+2l)^n, L+2l)}{\rho_{L+2l}(L+2l)^n},$$

where

$$\rho_L := \frac{\rho(L-2l)^n}{L^n} \to \rho \quad \text{as } L \to \infty.$$

Together with Corollary 3.3.3 we conclude that

$$e_0(\rho) \le \limsup_{L\to\infty} \frac{\langle \tilde{H}_L \rangle_\Psi}{\rho L^n},$$

for each periodic, normalized $\Psi \in \mathcal{F}_L$ with expected number of particles $\langle \mathcal{N} \rangle_\Psi = \rho L^n$.

Finally, we note that, with the periodic potential V_L, we have (in the sense of quadratic forms)

$$\tilde{H}_L = \sum_p p^2 a_p^+ a_p + \frac{1}{2L^n} \sum_{\substack{p,q,r,s \\ p+q=r+s}} \hat{V}_{p-r} a_p^+ a_q^+ a_r a_s, \tag{3.3.6}$$

where all sums are over Λ_L^* and where a_p^+ and a_p denote the bosonic creation and annihilation operators on $\mathcal{F}_L$ w.r.t. the plane wave $x \mapsto L^{-n/2} e^{ip\cdot x}$.

3.3.1 The Trial State

The state in (3.1.3) can be defined as follows. Fix $\rho, L > 0$ and set $N := \rho|\Lambda| = \rho L^n$. Then let

$$\Psi := \sum_\alpha f(\alpha)|\alpha\rangle \tag{3.3.7}$$

where $\{|\alpha\rangle\}_\alpha \subset \mathcal{F}$ is the orthonormal basis given by

$$|\alpha\rangle := \prod_{k\in\Lambda^*} \frac{1}{\sqrt{\alpha(k)!}} (a_k^+)^{\alpha(k)} |0\rangle,$$

for each $\alpha : \Lambda^* \to \mathbb{N}_0$ with $|\alpha| := \sum_{k\in\Lambda^*} \alpha(k) < \infty$. Note that, by the canonical commutation relations,

$$a_p|\alpha\rangle = \sqrt{\alpha(p)}|\alpha - \delta_p\rangle \quad \text{and} \quad a_p^+|\alpha\rangle = \sqrt{\alpha(p)+1}|\alpha + \delta_p\rangle, \tag{3.3.8}$$

for any $p \in \Lambda^*$, where $\delta_p(k) := \delta_{p,k}$. Let

$$\mathcal{M} := \big\{\alpha : \Lambda^* \to \mathbb{N}_0 : |\alpha| < \infty \text{ and } \alpha(-p) = \alpha(p) \text{ for each } p \in \Lambda^*\big\},$$

We define the coefficient function f in (4.2.1) by

$$f(\alpha) := \exp\left(N_0 + \sum_{p\neq 0} |\ln(1-c_p^2)|\right)^{-1/2} \cdot \left(\frac{N_0^{\alpha(0)}}{\alpha(0)!} \prod_{p\neq 0} c_p^{\alpha(p)}\right)^{1/2}, \tag{3.3.9}$$

for $\alpha \in \mathcal{M}$ and $f(\alpha) = 0$ otherwise. Here $c : \Lambda^* \backslash \{0\} \to (-1, 1)$ is to be chosen and

$$N_0 := N - \sum_{p \neq 0} \frac{c_p^2}{1 - c_p^2}. \tag{3.3.10}$$

It will be apparent later on that (3.3.10) is equivalent to the condition $\langle \Psi, \mathcal{N}\Psi \rangle = N$. We will assume that $c_{-p} = c_p$, for each p and clearly we also need some decay of c_p in order for the sums in (3.3.9) and (3.3.10) to converge. Given any operator A with a domain containing Ψ, we let $\langle A \rangle := \langle \Psi, A\Psi \rangle$ denote the expectation of A in the state Ψ. Most of the interaction terms in (3.3.6) have zero expectation in the state Ψ. In fact, since f vanishes outside $\mathcal{M}$ and since $\alpha(-p) = \alpha(p)$, for each $p \in \Lambda^*$ and each $\alpha \in \mathcal{M}$, it follows that only *pair* interactions terms where either $p = r$, $p = s$ or $p = -q$ have nonzero expectation in Ψ. Thus

$$\langle \tilde{H}_L \rangle = \sum_p p^2 \langle a_p^+ a_p \rangle + E_1 + E_2 + E_3,$$

where

$$E_1 := \frac{\hat{V}_0}{2|\Lambda|} \sum_{p,q} \langle a_p^+ a_q^+ a_p a_q \rangle, \quad E_2 := \frac{1}{2|\Lambda|} \sum_{p \neq q} \hat{V}_{p-q} \langle a_p^+ a_q^+ a_p a_q \rangle$$

and

$$E_3 := \frac{1}{2|\Lambda|} \sum_{p \neq \pm q} \hat{V}_{p-q} \langle a_p^+ a_{-p}^+ a_q a_{-q} \rangle.$$

Lemma 4.3.1 below provides us with all the relevant expectations in terms of N_0 and c_p. We introduce the notation

$$h_p := \frac{c_p^2}{1 - c_p^2} \quad \text{and} \quad s_p := \frac{c_p}{1 - c_p^2}.$$

Lemma 3.3.5. *Let $p, q \in \Lambda^*$ with $p \neq \pm q$ and $p \neq 0$. Then*

1. $\langle a_0^+ a_0 \rangle = N_0 = \langle a_0 a_0 \rangle$ *and* $\langle a_0^+ a_0 a_0^+ a_0 \rangle = N_0(N_0 + 1)$
2. $\langle a_p^+ a_p a_q^+ a_q \rangle = \langle a_p^+ a_p \rangle \cdot \langle a_q^+ a_q \rangle$
3. $\langle a_p^+ a_{-p}^+ a_q a_{-q} \rangle = \langle a_p^+ a_{-p}^+ \rangle \cdot \langle a_q a_{-q} \rangle$
4. $\langle a_p^+ a_p \rangle = h_p$
5. $\langle a_p^+ a_{-p}^+ \rangle = s_p$
6. $\langle a_p^+ a_p a_{\pm p}^+ a_{\pm p} \rangle = h_p(2h_p + 1)$

Proof. The identities are proved similarly, so we only show a few of them. By definition of Ψ and the relations (3.3.8), we have

$$\langle a_p^+ a_p \rangle = \sum_\alpha \alpha(p) |f(\alpha)|^2,$$

for any $p \in \Lambda^*$. Define the operation $\mathcal{A}^0\alpha := \alpha + \delta_0$ and $\mathcal{A}^p\alpha := \alpha + \delta_p + \delta_{-p}$, for $p \neq 0$. Notice that

$$f(\mathcal{A}^0\alpha) = N_0^{1/2}(\alpha(0)+1)^{-1/2}f(\alpha) \quad \text{and} \quad f(\mathcal{A}^p\alpha) = c_p f(\alpha).$$

We then have

$$\langle a_0^+ a_0 \rangle = \sum_{\alpha \in \mathcal{A}^0(\mathcal{M})} \alpha(0)|f(\alpha)|^2 = \sum_\beta (\beta(0)+1)|f(\mathcal{A}^0\beta)|^2 = N_0,$$

where we have also used that $\sum_\beta |f(\beta)|^2 = 1$ due to normalization. For $p \neq 0$ we get

$$\langle a_p^+ a_p \rangle = \sum_\beta (\beta(p)+1)|f(\mathcal{A}^p\beta)|^2 = c_p^2(\langle a_p^+ a_p \rangle + 1),$$

and solving for $\langle a_p^+ a_p \rangle$ yields 4. Also,

$$\langle a_p^+ a_{-p}^+ \rangle = \sum_\alpha \overline{f(\mathcal{A}^p\alpha)} f(\alpha)(\alpha(p)+1) = c_p(h_p+1) = s_p,$$

as claimed. □

Notice that, by Lemma 4.3.1,

$$\langle \mathcal{N} \rangle = \sum_p \langle a_p^+ a_p \rangle = N_0 + \sum_{p \neq 0} h_p,$$

and hence the condition $\langle \mathcal{N} \rangle = N$ is indeed equivalent to (3.3.10).

3.3.2 Computation of the Energy

Eventually we will choose c_p via the new variable

$$e_p := \frac{c_p}{1+c_p}, \quad h_p = \frac{e_p^2}{1-2e_p}, \quad s_p = \frac{e_p(1-e_p)}{1-2e_p}.$$

Note that the constraint $|c_p| < 1$ is equivalent to $e_p < 1/2$. In Lemma 3.3.6 below we calculate the energy $\langle \tilde{H}_L \rangle$ per particle in the thermodynamic limit

$$E(\rho) := \lim_{L\to\infty} \frac{\langle \tilde{H}_L \rangle}{\rho L^n}.$$

For this reason, it is convenient to assume that e_p is independent of L, i.e. we assume that c is defined on $\mathbb{R}^n \backslash \{0\}$ rather than on $\Lambda^* \backslash \{0\}$. We will also employ the fact that for any continuous function $F \in L^1(\mathbb{R}^n)$, decaying faster than $|p|^{-n-\varepsilon}$ at infinity, for some $\varepsilon > 0$, we have the convergence

$$\lim_{L\to\infty} \frac{1}{L^n} \sum_{p \in \Lambda^*} F(p) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} F(p)\, dp. \tag{3.3.11}$$

We denote the scattering solution by $1-w$ and set

$$\varphi := Vw \quad \text{and} \quad g := V - \varphi = V(1-w).$$

Note that $\hat{g}_0 > 0$, unless V is trivial. Though w is not integrable, it follows from the scattering equation (4.B.2) that, as tempered distribution, $\hat{w}$ equals the function $p \mapsto \hat{g}_p/(2p^2)$. We shall abuse notation slightly by denoting

$$\hat{w}_p := \frac{\hat{g}_p}{2p^2}.$$

Lemma 3.3.6. *Suppose that $e : \mathbb{R}^n \backslash \{0\} \to (-\infty, 1/2)$ is continuous and integrable with fast decay. Then*

$$E(\rho) = \frac{\hat{g}_0}{2}\rho + Q + \tilde{Q} + \Omega,$$

where

$$Q := \frac{1}{2(2\pi)^n \rho} \int p^2 \left[\frac{e_p^2 + 2\rho \hat{w}_p e_p}{1 - 2e_p} + (\rho \hat{w}_p)^2 \right] dp,$$

$$\tilde{Q} := \frac{2}{(2\pi)^n} \int \hat{\varphi}_p h_p \, dp,$$

$$\Omega := \frac{1}{2(2\pi)^{2n}\rho} \int \int \left[\hat{V}_{p-q}(e_p + \rho \hat{w}_p)(e_q + \rho \hat{w}_q) + 2(\hat{V}_{p-q} - \hat{V}_p) s_p h_q - 2\hat{V}_p h_p h_q \right] dp \, dq.$$

Proof. By Lemma 4.3.1, the kinetic energy is simply

$$\sum_p p^2 \langle a_p^+ a_p \rangle = \sum_{p \neq 0} p^2 h_p = \sum_{p \neq 0} \frac{p^2 e_p^2}{1 - 2e_p}.$$

Using commutation relations, Lemma 4.3.1 and (3.3.10), we find that

$$E_1 = \frac{\hat{V}_0}{2|\Lambda|} \left(\sum_{p,q} \langle a_p^+ a_p a_q^+ a_q \rangle - \sum_p \langle a_p^+ a_p \rangle \right) = \frac{\hat{V}_0}{2|\Lambda|} \left(N^2 + \sum_{p \neq 0} h_p(h_p + 1) \right),$$

where the last sum comes from the special cases $p = \pm q$. Note that contributions like that will vanish in the energy per particle in the thermodynamic limit. Similarly,

$$\begin{aligned} E_2 &= \frac{N_0}{|\Lambda|} \sum_{p \neq 0} \hat{V}_p h_p + \frac{1}{2|\Lambda|} \sum_{p \neq 0} \hat{V}_{2p} h_p (2h_p + 1) + \frac{1}{2|\Lambda|} \sum_{\substack{p,q \neq 0 \\ p \neq \pm q}} \hat{V}_{p-q} h_p h_q \\ &= \sum_{p \neq 0} \rho \hat{V}_p h_p - \frac{1}{|\Lambda|} \sum_{p,q \neq 0} \hat{V}_p h_p h_q + \frac{1}{2|\Lambda|} \sum_{p \neq 0} \hat{V}_{2p} h_p (2h_p + 1) + \frac{1}{2|\Lambda|} \sum_{\substack{p,q \neq 0 \\ p \neq \pm q}} \hat{V}_{p-q} h_p h_q, \end{aligned}$$

and also

$$E_3 = \sum_{p \neq 0} \rho \hat{V}_p s_p - \frac{1}{|\Lambda|} \sum_{p,q \neq 0} \hat{V}_p s_p h_q + \frac{1}{2|\Lambda|} \sum_{\substack{p,q \neq 0 \\ p \neq \pm q}} \hat{V}_{p-q} s_p s_q.$$

Thus, in the limit $L \to \infty$,

$$\begin{aligned} E(\rho) &= \frac{\hat{V}_0\rho}{2} + \frac{1}{(2\pi)^n\rho}\int \frac{p^2e_p^2+\rho\hat{V}_pe_p}{1-2e_p}\,dp + \frac{1}{2(2\pi)^{2n}\rho}\int\int \hat{V}_{p-q}s_ps_q - 2\hat{V}_ps_ph_q\,dp\,dq \\ &+ \frac{1}{2(2\pi)^{2n}\rho}\int\int \hat{V}_{p-q}h_ph_q - 2\hat{V}_ph_ph_q\,dp\,dq. \end{aligned}$$

By the relation $e_p = s_p - h_p$ we have

$$\int\int \hat{V}_{p-q}s_ps_q - 2\hat{V}_ps_ph_q\,dp\,dq = \int\int \hat{V}_{p-q}(e_pe_q - h_ph_q) + 2(\hat{V}_{p-q}-\hat{V}_p)s_ph_q\,dp\,dq$$

and hence

$$\begin{aligned} E(\rho) &= \frac{\hat{V}_0\rho}{2} + \frac{1}{(2\pi)^n\rho}\int \frac{p^2e_p^2+\rho\hat{V}_pe_p}{1-2e_p}\,dp + \frac{1}{2(2\pi)^{2n}\rho}\int\int \hat{V}_{p-q}e_pe_q\,dp\,dq \\ &+ \frac{1}{(2\pi)^{2n}\rho}\int\int (\hat{V}_{p-q}-\hat{V}_p)s_ph_q - \hat{V}_ph_ph_q\,dp\,dq. \end{aligned}$$

Now, using $(2\pi)^n\hat{\varphi} = \hat{V} * \hat{w}$, (3.2.6) and $V = g + \varphi$, we get

$$\frac{\hat{V}_0\rho}{2} = \frac{\hat{g}_0\rho}{2} + \frac{\rho}{2(2\pi)^n}\int \hat{V}_p\hat{w}_p\,dp = s_na^{n-2}\rho + \frac{\rho}{2(2\pi)^n}\int \hat{g}_p\hat{w}_p\,dp + \frac{\rho}{2(2\pi)^n}\int \hat{\varphi}_p\hat{w}_p\,dp$$

and also

$$\begin{aligned} \frac{1}{2(2\pi)^{2n}\rho}\int\int \hat{V}_{p-q}e_pe_q\,dp\,dq &= \frac{1}{2(2\pi)^{2n}\rho}\int\int \hat{V}_{p-q}(e_p+\rho\hat{w}_p)(e_q+\rho\hat{w}_q)\,dp\,dq \\ &- \frac{1}{(2\pi)^n}\int \hat{\varphi}_pe_p\,dp - \frac{\rho}{2(2\pi)^n}\int \hat{\varphi}_p\hat{w}_p\,dp. \end{aligned}$$

Combining terms yields the desired. □

In [4] the function e_p is chosen as the pointwise minimizer of the sum of integrands in Q and $\tilde{Q}$. However, it turns out that including the latter in the minimization problem does not lower the energy significantly. In fact, the calculation of Yau-Yin [25] suggests that $\tilde{Q}$ is really not present in the ground state energy, but should rather be cancelled by a term 'missing' in the energy of our trial state. Thus we will choose e_p to minimize the simpler expression

$$m_p := \frac{e_p^2 + 2\rho\hat{w}_pe_p}{1-2e_p}.$$

This yields

$$-e_p^2 + e_p + \rho\hat{w}_p = 0, \quad e_p = \frac{1}{2}\left(1 - \sqrt{1+4\rho\hat{w}_p}\right) \tag{3.3.12}$$

and

$$m_p = \frac{(1-2e_p)(-e_p-\rho\hat{w}_p) + (-e_p^2+e_p+\rho\hat{w}_p)}{1-2e_p} = \frac{1}{2}\big(\sqrt{1+4\rho\hat{w}_p} - 1 - 2\rho\hat{w}_p\big),$$

provided $1 + 4\rho\hat{w}_p \geq 0$. Note however that, since $\hat{g}$ is continuous, $\hat{g}_0 > 0$ and $\hat{g}_p \to 0$ as $|p| \to \infty$, it follows that $\hat{w}_p$ is bounded from below, and hence

$$\liminf_{\rho\to 0} \left[\inf_{p\neq 0} (1 + 4\rho\hat{w}_p) \right] \geq 1.$$

With the choice in (4.5.3) we have

$$Q = \frac{1}{2(2\pi)^n\rho} \int p^2 \Phi(\rho\hat{w}_p)\, dp, \tag{3.3.13}$$

where

$$\Phi(t) := \sqrt{1+4t} + 2t^2 - 2t - 1. \tag{3.3.14}$$

Finally, we note that $|e_p| \leq \rho|\hat{w}_p|$, for $|p| \gg \rho^{1/2}$, and hence e inherits decay from $\hat{g}$.

3.3.3 Estimates

In this section we estimate the integrals from Lemma 3.3.6 in the limit $\rho \to 0$, given the particular choice in (4.5.3). We begin with the term Q, and in fact we will derive asymptotics of order up to $\sim n/2$ with coefficients, all except one, given in terms of integrals of $\hat{w}_p$ (see also Table 1 below). We stress, however, that the physical relevance of these higher order asymptotics remains to be understood. In fact, while the main contribution in dimension three and four comes from Q, we believe that Ω and Q are of the same leading order in dimension $n \geq 5$.

Lemma 3.3.7. *In dimension $n = 3$,*

$$Q = (4\pi a\rho)\cdot \frac{128}{15\sqrt{\pi}} Y^{1/2} + o(\rho^{3/2}) \quad \textit{and} \quad Q \leq (4\pi a\rho)\cdot\frac{128}{15\sqrt{\pi}} Y^{1/2}.$$

In dimension $n \geq 4$,

$$Q = \sum_{m=3}^{\lceil n/2\rceil} c_m \rho^{m-1} + c_{n/2+1}\Big(s_n a^{n-2}\rho Y^{n/2-1} |\ln Y|\Big) + \mathcal{O}(\rho^{n/2}),$$

where the error term depends on V and where $c_m = 0$ if $m \notin \mathbb{N}$,

$$c_m := \frac{\Phi^{(m)}(0)}{2(2\pi)^n m!} \int_{\mathbb{R}^n} p^2 \hat{w}_p^m, \quad m \leq (n+1)/2,$$

and

$$c_{n/2+1} := \frac{\Phi^{(n/2+1)}(0) |\mathbb{S}^{n-1}|^{n/2+1} (n-2)^{n/2}}{4(2\pi)^n (n/2+1)!}.$$

The function Φ is given in (4.5.6).

Proof. We first consider the case $n = 3$. Let $\varepsilon = (\hat{g}_0\rho)^{1/2}$. By a change of variables $p \mapsto \varepsilon p$, continuity of $\hat{g}$ and the dominated convergence theorem we have

$$\rho^{-3/2} Q = \frac{\hat{g}_0^{5/2}}{2(2\pi)^3} \int_{\mathbb{R}^3} p^2 \Phi\left(\frac{\hat{g}_{\varepsilon p}}{2p^2\hat{g}_0}\right) dp \to \frac{\hat{g}_0^{5/2}}{2(2\pi)^3} \int_{\mathbb{R}^3} p^2 \Phi\left(\frac{1}{2p^2}\right) dp \tag{3.3.15}$$

as $\rho \to 0$. A direct calculation then yields

$$Q = (4\pi a\rho) \cdot \frac{128}{15\sqrt{\pi}} Y^{1/2} + o(\rho^{3/2}). \tag{3.3.16}$$

The explicit upper bound claimed in the lemma can be obtained from the same calculation with the additional information that Φ is increasing and $\hat{g}_p \leq \hat{g}_0$. In [4] the estimate is done more carefully and shows that (3.3.16) holds with $o(\rho^{3/2})$ replaced by $\mathcal{O}(\rho^2 |\ln \rho|)$. In higher dimensions the asymptotics of Q is more subtle, due to the fact that the latter integral in (3.3.15) becomes divergent! That is, we cannot replace $\hat{g}_p$ by $\hat{g}_0$, because we need the decay of $\hat{g}$ in order for the integral to converge. However, from the asymptotics of Φ we get some information. First notice that $\Phi(t)t^{-2} \to 2$ as $t \to \infty$, and in fact, $\Phi(t) \leq 2t^2$, for each $t \geq -1/4$. Hence

$$\begin{aligned} Q'_\varepsilon &:= \frac{1}{2(2\pi)^n \rho} \int_{|p|\leq\varepsilon} p^2 \Phi(\rho \hat{w}_p)\, dp \leq \frac{1}{2(2\pi)^n \rho} \int_{|p|\leq\varepsilon} p^2 2(\rho \hat{w}_p)^2\, dp \\ &\leq \frac{\hat{g}_0^2 \rho}{4(2\pi)^n} \int_{|p|\leq\varepsilon} p^{-2}\, dp = C a^{n-2} \rho Y^{n/2-1}, \end{aligned}$$

where we have inserted $\hat{g}_0 = 2 s_n a^{n-2}$. To estimate $Q_\varepsilon := Q - Q'_\varepsilon$, we expand Φ to the $(k-1)$'th order around $t = 0$, where k is the smallest integer such that $2k \geq n+3$. Since $\Phi(0) = \Phi'(0) = \Phi''(0) = 0$, we have

$$\Phi(t) = b_3 t^3 + \ldots + b_{k-1} t^{k-1} + \mathcal{O}(t^k),$$

where $b_m := \Phi^{(m)}(0)/m!$. Correspondingly we have the expansion

$$Q_\varepsilon = Q_\varepsilon^{(3)} + \ldots + Q_\varepsilon^{(k-1)} + \mathcal{E},$$

where

$$Q_\varepsilon^{(m)} := \frac{b_m}{2(2\pi)^n \rho} \int_{|p|>\varepsilon} p^2 (\rho \hat{w}_p)^m\, dp,$$

and where

$$|\mathcal{E}| \leq C\rho^{-1} \int_{|p|>\varepsilon} |\rho \hat{w}_p|^k\, dp \leq C \hat{g}_0^k \rho^{k-1} \int_{|p|>\varepsilon} p^{2-2k}\, dp = C a^{n-2} \rho Y^{n/2-1}.$$

If $m < n/2+1$, then $p^2 \hat{w}_p^m$ is integrable at $p = 0$, and we have

$$Q_\varepsilon^{(m)} = \frac{b_m \rho^{m-1}}{2(2\pi)^n} \int p^2 \hat{w}_p^m\, dp + \mathcal{O}\big(a^{n-2} \rho Y^{n/2-1}\big).$$

Notice that if n is odd, then $k = (n+3)/2$, and hence $m < n/2+1$, for each $m \leq k-1$. In equal dimension there is a $m = n/2+1$ term:

$$\begin{aligned} Q_\varepsilon^{(m)} &= \frac{b_m}{2(2\pi)^n \rho} \int_{\varepsilon<|p|\leq 1} p^2 (\rho \hat{w}_p)^m\, dp + \mathcal{O}(\rho^{m-1}) \\ &= \frac{b_m}{2(2\pi)^n \rho} \int_{\varepsilon<|p|\leq 1} p^2 \left(\frac{\hat{g}_0}{2p^2}\right)^m dp + \mathcal{O}(\rho^{m-1}), \end{aligned}$$

n	Q		
3	$\rho^{3/2}$	$\mathcal{O}(\rho^2\lvert\ln\rho\rvert)$	
4	$\rho^2\lvert\ln\rho\rvert$	$\mathcal{O}(\rho^2)$	
5	ρ^2	$\mathcal{O}(\rho^{5/2})$	
6	ρ^2	$\rho^3\lvert\ln\rho\rvert$	$\mathcal{O}(\rho^3)$
7	ρ^2	ρ^3	$\mathcal{O}(\rho^{7/2})$
$\vdots$	$\vdots$		

Table 3.1: Qualitative expansion of Q in the first few dimensions.

where the errors depend on V, and where we have used Lipschitz continuity of $\hat{g}$ to replace $\hat{g}_p$ with $\hat{g}_0$ in the second estimate. Now, by inserting $\hat{g}_0 = 2s_n a^{n-2}$, we get

$$Q_\varepsilon^{n/2+1} = s_n a^{n-2}\rho\frac{b_{n/2+1}|\mathbb{S}^{n-1}|^{n/2+1}(n-2)^{n/2}}{4(2\pi)^n}Y^{n/2-1}|\ln Y| + \mathcal{O}(\rho^{n/2}),$$

where we have artificially replaced $|\ln(\hat{g}_0\rho)|$ by $|\ln Y|$ at the cost of an error of order $\rho^{n/2}$, depending on V. In particular, with $b_3 = 4$ and $|\mathbb{S}^3| = 2\pi^2$, we have

$$Q_2^{(3)} = (4\pi^2 a^2\rho)\cdot 2\pi^2 Y|\ln Y| + \mathcal{O}(\rho^2),$$

which is the term present in four dimensions. □

In table 1 we have listed the powers of ρ in the expansion of Q up to dimension $n = 7$. Whether the expansion of $e_0(\rho)$ has this structure too remains to be clarified.

Lemma 3.3.8.

$$\Omega(\rho) = \begin{cases} \mathcal{O}(\rho^2|\ln\rho|) & n = 3 \\ \mathcal{O}(\rho^2) & n \geq 4 \end{cases}$$

Proof. Using $|\hat{V}_p| \leq \hat{V}_0$, Lipschitz continuity of $\hat{V}$ and the relation in (4.5.3), we have

$$|\Omega| \leq C_V\rho^{-1}\Big\{\Big(\int e_p^2\,dp\Big)^2 + \Big(\int |s_p|\,dp\Big)\Big(\int h_q|q|\,dq\Big) + \Big(\int h_p\,dp\Big)^2\Big\}.$$

Notice the asymptotics

$$h_p = \frac{1}{2}\Big(\frac{1+2\rho\hat{w}_p}{\sqrt{1+4\rho\hat{w}_p}} - 1\Big) = \begin{cases} \mathcal{O}\big(\sqrt{\rho\hat{w}_p}\big) & \text{as } |\rho\hat{w}_p| \to \infty \\ \mathcal{O}\big(\rho^2\hat{w}_p^2\big) & \text{as } |\rho\hat{w}_p| \to 0 \end{cases}.$$

In fact, $h_p \leq C\rho^2\hat{w}_p^2$ for each $p \neq 0$, provided ρ is sufficiently small. In dimension $n \geq 5$ we then simply have

$$\int h_p\,dp = \mathcal{O}\big(\rho^2\|\hat{w}\|_2^2\big).$$

Otherwise we split the integral into two parts

$$\int h_p\,dp \le C\left[\int_{|p|\le\varepsilon}(\rho\hat{w}_p)^{1/2}\,dp + \int_{|p|>\varepsilon}(\rho\hat{w}_p)^2\,dp\right] = I_1 + I_2$$

where $\varepsilon := (a\rho)^{1/2}$. Since $\hat{g}_p \le \hat{g}_0 = 2s_n a^{n-2}$, it follows that $I_1 = \mathcal{O}(\rho Y^{n/2-1})$. In dimension $n = 3$ we again use $|\hat{g}_p| \le \hat{g}_0$ to obtain $I_2 = \mathcal{O}(\rho Y^{1/2})$, and in four dimensions we get a logarithmic term,

$$I_2 \le C\rho Y|\ln Y| + C_V\rho^2.$$

In total,

$$\int h_p\,dp \le \begin{cases} C\rho Y^{1/2} & n=3 \\ C\rho Y|\ln Y| + C_V\rho^2 & n=4 \\ C_V\rho^2 & n\ge 5 \end{cases}. \tag{3.3.17}$$

By repeating the above estimates with an additional factor $|p|$ in the integrands, we see that

$$\int |p|h_p\,dp \le \begin{cases} C_V\rho^2|\ln\rho| & n=3 \\ C_V\rho^2 & n\ge 4 \end{cases}.$$

The integral of e_p^2 is estimated similarly to h_p and in fact (3.3.17) holds with h_p replaced by e_p^2. Finally, since

$$s_p = \frac{-\rho\hat{w}_p}{\sqrt{1+4\rho\hat{w}_p}},$$

we see that

$$\int |s_p|\,dp = \mathcal{O}(\rho),$$

for any $n \ge 3$, and we are done. □

Remark 3.3.9. *From the estimate* (3.3.17) *and* $|\hat{\varphi}_p| \le \hat{\varphi}_0$ *it follows that*

$$\tilde{Q}(p) \le \begin{cases} C\gamma a\rho Y^{1/2} & n=3 \\ C\gamma a^2\rho Y|\ln Y| + C_V\rho^2 & n=4 \\ C_V\rho^2 & n\ge 5 \end{cases},$$

where $\gamma := \hat{\varphi}_0/\hat{g}_0$.

In order to finish the proof of Theorem 3.3.1 we only need to show that

$$\gamma \le C\|V\|_\infty^{1-2/n}\|V\|_1^{2/n}. \tag{3.3.18}$$

However, from the representation (3.2.5) and the fact that $\varphi \ge 0$ it follows that

$$\varphi = Vw = \frac{1}{2}V\Gamma g = \frac{1}{2}V(\Gamma V - \Gamma\varphi) \le \frac{1}{2}V\Gamma V.$$

Then by Hölder's inequality and the Hardy-Littlewood-Sobolev inequality,

$$\|V\Gamma V\|_1 \le \|V\|_p \cdot \|\Gamma V\|_{p'} \le C\|V\|_p^2 \le C\|V\|_\infty^{1-2/n} \cdot \|V\|_1^{1+2/n}$$

where $p := 2n/(n+2)$ and $p' := p/(p-1)$ is the dual exponent of p. On the other hand $\hat{g}_0 = \hat{V}_0 - \hat{\varphi}_0 \ge \|V\|_1$, and (3.3.18) follows.

Acknowledgements

A. Aaen was partially supported by the Lundbeck Foundation and the European Research Council under the European Community's Seventh Framework Program (FP7/2007–2013)/ERC grant agreement 202859.

3.A Equivalence of Ensembles

In this section we prove Lemma 3.3.2. We will see that the canonical and grand canonical energies are related via the Legendre transform, and in order for this to be well-behaved globally, it is convenient to have high density bounds on the ground state energy. A trivial upper bound to $E_0(N, L)$ with periodic boundary conditions is obtained by calculating the energy of the constant function:

$$E_0(N, L) \le \frac{N(N-1)}{2|\Lambda|} \int V(x)\, dx.$$

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

$$e_0(\rho) \le \frac{\hat{V}_0}{2}\rho. \tag{3.A.1}$$

In the following lemma we derive a simple lower bound to $E_0(N, L)$ under the assumption that V is uniformly strictly positive in a neighborhood of the origin. Due to lack of space, this forces a large fraction of the particles to interact.

Lemma 3.A.1. *Suppose that $V \ge \varepsilon \chi_{B(0,2R)}$, for some $\varepsilon, R > 0$. Then*

$$E_0(N, L) \ge C\varepsilon R^n \frac{N^2}{|\Lambda|} - \frac{N}{2}V(0), \tag{3.A.2}$$

for some constant $C > 0$ depending only on the dimension.

Proof. We will simply discard the kinetic energy and show that the total interaction is pointwise bounded from below by the RHS in (3.A.2). Let $\chi_R = \chi_{B(0,R)}$. By Jensen's inequality we have

$$\left(\int_\Lambda \sum_{j=1}^N \chi_R(x_j - z) \frac{dz}{|\Lambda|} \right)^2 \le \frac{1}{|\Lambda|} \sum_{j,k} \int_\Lambda \chi_R(x_j - z)\chi_R(x_k - z)\, dz.$$

However, the triangle inequality shows that

$$\chi_R(x_j - z)\chi_R(x_k - z) \leq \chi_{2R}(x_j - x_k)\chi_R(x_k - z),$$

and hence

$$\begin{aligned}\left(\int_\Lambda \sum_{j=1}^N \chi_R(x_j - z)\, \frac{dz}{|\Lambda|}\right)^2 &\leq \frac{v_n R^n}{|\Lambda|} \sum_{j,k} \chi_{2R}(x_j - x_k) \leq \frac{v_n R^n}{\varepsilon|\Lambda|} \sum_{j,k} V(x_j - x_k) \\ &= \frac{v_n R^n}{\varepsilon|\Lambda|}\left(2\sum_{j<k} V(x_j - x_k) + NV(0)\right),\end{aligned}$$

where v_n denotes the volume of the unit ball in $\mathbb{R}_n$. The result now follows by noting that

$$\int_\Lambda \sum_{j=1}^N \chi_R(x_j - z)\, dz \geq N v_n 2^{-n} R^n,$$

where the inequality and the factor 2^{-n} comes from the situation where x_j is located close the corner of the box. □

Recall the notation in (3.3.4) and (3.3.5) for the ground state energy per volume. As a technical convenience we extend, for fixed $L > 0$, the mapping $N \mapsto E_0(N, L)$ to $[0, \infty)$, as a piecewise linear function, by setting $E(0, L) = 0$ and

$$E_0(N + \sigma, L) = (1 - \sigma)E_0(N, L) + \sigma E_0(N + 1, L), \quad \sigma \in [0, 1]. \tag{3.A.3}$$

Note that, as a consequence of Lemma 3.A.1 we have the lower bounds

$$e_L(\rho) \geq C_1\rho^2 - C_2\rho \quad \text{and} \quad e(\rho) \geq C_1\rho^2 - C_2\rho, \tag{3.A.4}$$

for constants $C_1, C_2 > 0$ depending on V.

Since each N-particle sector is naturally imbedded in the Fock space, it follows that $E_0^{\mathrm{GC}}(N, L) \leq E_0(N, L)$. We remark that in case N is not a natural number, the inequality follows from the convention (3.A.3) by considering the combination

$$\Psi := \sqrt{1 - \sigma}\Psi_{\lfloor N \rfloor} + \sqrt{\sigma}\Psi_{\lceil N \rceil}$$

of arbitrary $\lfloor N \rfloor$-particle and $\lceil N \rceil$-particles states, where $\sigma := N - \lfloor N \rfloor$. In order to prove Lemma 3.3.2, we therefore only need to show that

$$\liminf_{L\to\infty} e_L^{GC}(\rho) \geq e(\rho). \tag{3.A.5}$$

We introduce a chemical potential $\mu \geq 0$ and notice that, for any normalized $\Psi = (\Psi_0, \Psi_1, \ldots) \in \mathcal{F}$ with $\langle \Psi, \mathcal{N}\Psi \rangle \geq \rho L^n$ we have the lower bound

$$\begin{aligned}\frac{\langle \Psi, H_L\Psi \rangle}{L^n} &= \frac{1}{L^n}\left[\mu\langle \Psi, \mathcal{N}\Psi \rangle + \langle \Psi, (H_L - \mu\mathcal{N})\Psi \rangle\right] \\ &\geq \mu\rho + \sum_{N=0}^\infty \|\Psi_N\|^2 \left[e_L(N/L^n) - \mu\frac{N}{L^n}\right] \\ &\geq \mu\rho + f_L(\mu),\end{aligned}$$

where $f_L := -e_L^*$ and where

$$g^*(\mu) := \sup_{\rho \geq 0} \left[\mu\rho - g(\rho)\right],$$

denotes the Legendre Transform of any function $g : [0, \infty) \to \mathbb{R}$, and for $\mu \geq 0$ such that the supremum is finite. We will employ the well-known fact [21] that the Legendre transform is involute on convex functions, meaning that $(g^*)^* = g^*$. The inequality (3.A.5) will then follow, provided we can show the convergence

$$\lim_{L\to\infty} f_L(\mu) = f(\mu) := -e^*(\mu),$$

for each $\mu \geq 0$. Now, by definition,

$$f_L(\mu) \leq e(\rho) - \mu\rho + [e_L(\rho) - e(\rho)],$$

and hence

$$\limsup_{L\to\infty} f_L(\mu) \leq e(\rho) - \mu\rho,$$

for each $\rho \geq 0$. It follows that

$$\limsup_{L\to\infty} f_L(\mu) \leq f(\mu).$$

For the lower bound we employ the following lemma.

Lemma 3.A.2. *Suppose that V is compactly supported with, say, supp$(V) \subset B(0, R)$. Then*

$$e_L(\rho) \geq (1 + R/L)^n e(\rho[1 + R/L]^{-n})$$

for each $\rho, L > 0$.

Proof. By convexity of $e(\rho)$ we may assume that $N := \rho L^n$ is an integer. Let $k \in \mathbb{N}$ and put $L' = k(L+R)$.We can place $M := k^n$ copies of the box Λ_L inside the larger box $\Lambda_{L'}$ with separation R between neighboring boxes. From an N-particle trial state Ψ in Λ_L we can construct a trial state with MN particles by placing independent particles in each of the M boxes, each with state Ψ. Because of the Dirichlet boundary condition, this gives a trial state on $\Lambda_{L'}$ by extending Ψ by zero and, due to the separation, particles in different boxes do not interact. Minimizing over Ψ yields

$$e_L(\rho) \geq (1 + R/L)^n e_{L'}(\rho[1 + R/L]^{-n}).$$

This estimate holds for each $k \in \mathbb{N}$, so the result follows by taking the limit $k \to \infty$. □

By Lemma 3.A.2 we have

$$\begin{aligned} e_L(\rho) - \mu\rho &\geq e(\rho_L) - \mu\rho \\ &= [1 + R/L]^n (e(\rho_L) - \mu\rho_L) + \varepsilon_L \\ &\geq [1 + R/L]^n f(\mu) + \varepsilon_L, \end{aligned}$$

where

$$\rho_L := \rho[1+R/L]^{-n} \quad \text{and} \quad \varepsilon_L := e(\rho_L)(1-[1+R/L]^n).$$

Now notice that, by (3.A.4),

$$f_L(\mu) = \inf_{\rho\in[0,\rho_\mu]}[e_L(\rho) - \mu\rho],$$

for some $\rho_\mu > 0$. From the upper bound (3.A.1), we then have

$$f_L \geq [1+R/L]^n f(\mu) + C\rho_\mu^2(1-[1+R/L]^n),$$

and consequently

$$\liminf_{L\to\infty} f_L(\mu) \geq f(\mu),$$

as desired.

3.B Dyson's Upper Bound

In this appendix we prove Dyson's upper bound, which we employed in the proof of Theorem 3.2.2. The result in fact holds in any dimension, including $n = 1, 2$. Our calculation follows closely [3] and [11].

Theorem 3.B.1. *Suppose that $f \in H^1_{loc}(\mathbb{R}^n)$ is radially symmetric and satisfies*

$$0 \leq f \leq 1 \quad \textit{and} \quad f' \geq 0.$$

Define

$$I = \int (1-f(x)^2)\, dx, \quad K = \int f(x)|\nabla f(x)|\, dx$$

and

$$J = \int |\nabla f(x)|^2 + \frac{1}{2}V(x)f(x)^2\, dx.$$

Let $N \geq 2$, $L > 0$ and set $\rho = N/L^n$. Suppose that $\rho I < 1$. Then

$$\frac{E_0(N,L)}{N} \leq \frac{J\rho + \frac{2}{3}(K\rho)^2}{(1-I\rho)^2}, \tag{3.B.1}$$

where periodic boundary conditions have been imposed on the left-hand side.

Proof. We construct a trial state with energy bounded by N times the right-hand side in (3.B.1). Let

$$\Psi := F_2 \cdot F_3 \cdots F_N,$$

where $F_i := f(t_i)$,

$$t_i := \min_{1\leq j<i} d(x_i, x_j) \quad \text{and} \quad d(x,y) := \min_{m\in\mathbb{Z}^n} |x-y-mL|, \quad \text{for } x, y \in \mathbb{R}^n.$$

Notice that Ψ is continuous and periodic and that t_i and F_i only depend on the variables $x_1, \dots, x_i$. Also, $d(x,y) = |x-y|$ whenever $(x-y) \in \Lambda$ and, for almost all $(x_1, \dots, x_N) \in$

$\mathbb{R}^{n\cdot N}$, there exists a unique $j < i$ such that $t_i = d(x_i, x_j)$. For each i the function F_i is weakly differentiable with

$$|\nabla_k F_i| = \varepsilon_{ik} f'(t_i), \tag{3.B.2}$$

where

$$\varepsilon_{ik}(x_1, \ldots, x_N) := \begin{cases} 1 & \text{for } k = i \text{ or } t_i = d(x_i, x_k) \\ 0 & \text{otherwise} \end{cases}.$$

Moreover, by the product rule, Ψ is weakly differentiable with

$$\nabla_k \Psi = \sum_{i=2}^{N} \Psi F_i^{-1} \nabla_k F_i. \tag{3.B.3}$$

where the expression ΨF_i^{-1} is simply a shorthand for $F_2 \ldots F_{i-1} F_{i+1} \ldots F_N$. Thus we have

$$|\nabla_k \Psi| \leq \sum_{i=2}^{N} \Psi F_i^{-1} f'(t_i) \varepsilon_{ik},$$

and hence

$$\sum_{k=1}^{N} |\nabla_k \Psi|^2 \leq \sum_{i=2}^{N} \sum_{j=2}^{N} \sum_{k=1}^{N} \varepsilon_{ik} \varepsilon_{jk} (\Psi F_i^{-1})(\Psi F_j^{-1}) f'(t_i) f'(t_j).$$

We divide the above sum into two parts; one containing terms with $i = j$ and one containing terms with $i \neq j$. Since the summands are symmetric in i and j, the part with $i \neq j$ equals 2 times the part with, say, $j < i$. Moreover, when $j < i$ only terms with $k \leq j$ can be nonzero. For the part with $i = j$ we notice that $\sum_k \varepsilon_{ik}^2 = 2$ almost everywhere. It follows that

$$\sum_{k=1}^{N} |\nabla_k \Psi|^2 \leq 2 \sum_{i=2}^{N} (\Psi F_i^{-1})^2 f'(t_i)^2 + 2 \sum_{k \leq j < i} \varepsilon_{ik} \varepsilon_{jk} (\Psi F_i^{-1})(\Psi F_j^{-1}) f'(t_i) f'(t_j).$$

Thus we have $\langle \Psi, H_{N,L} \Psi \rangle \leq E_1 + E_2$, where

$$E_1 := \sum_{i=2}^{N} \left(\int \Psi^2 \right)^{-1} \left(\int 2(\Psi F_i^{-1})^2 f'(t_i)^2 + \sum_{j=1}^{i-1} V(x_i - x_j) \Psi^2 \right)$$

and

$$E_2 := 2 \sum_{k \leq j < i} \left(\int \Psi^2 \right)^{-1} \int \varepsilon_{ik} \varepsilon_{jk} (\Psi F_i^{-1})(\Psi F_j^{-1}) f'(t_i) f'(t_j).$$

The integrands in E_1 and E_2 involve the functions F_i both in the numerator and the denominator, so we need both upper and lower bounds on these. For $p > i, j \geq 2$ we define

$$F_{p,i} = \min_{\substack{k<p \\ k \neq i}} f(d(x_p, x_k)), \qquad F_{p,ij} = \min_{\substack{k<p \\ k \neq i,j}} f(d(x_p, x_k)).$$

Notice that $F_{p,i}$ does not depend on x_i, and similarly $F_{p,ij}$ does not depend on x_i and x_j. Since f is increasing and $0 \leq f \leq 1$,

$$F_{p,i}^2 f(d(x_p,x_i))^2 \leq F_p^2 \leq F_{p,i}^2 \quad \text{and} \quad F_{p,ij}^2 f(d(x_p,x_i))^2 f(d(x_p,x_j))^2 \leq F_p^2 \leq F_{p,ij}^2.$$

Hence, for $2 \leq j < i \leq N$, we have the upper bound

$$\left(F_{j+1}^2 \cdots F_{i-1}^2\right)\left(F_{i+1}^2 \cdots F_N^2\right) \leq \left(F_{j+1,j}^2 \cdots F_{i-1,j}^2\right)\left(F_{i+1,ij}^2 \cdots F_{N,ij}^2\right) \tag{3.B.4}$$

and the lower bound

$$\begin{aligned} F_j^2 \cdots F_N^2 &\geq \prod_{p=1}^{j-1} f(d(x_p,x_j))^2 \prod_{p=j+1}^{i-1} F_{p,j}^2 f(d(x_p,x_j))^2 \\ &\times \prod_{p=1}^{i-1} f(d(x_p,x_i))^2 \prod_{p=i+1}^{N} F_{p,ij}^2 f(d(x_p,x_i))^2 f(d(x_p,x_j))^2 \\ &= \left(F_{j+1,j}^2 \cdots F_{i-1,j}^2\right)\left(F_{i+1,ij}^2 \cdots F_{N,ij}^2\right) \qquad (3.B.5) \\ &\times \prod_{p=1,p\neq i,j}^{N} f(d(x_p,x_j))^2 \prod_{p=1,p\neq i}^{N} f(d(x_p,x_i))^2. \end{aligned}$$

In the lower bound we have also employed the fact that

$$F_j^2 \geq \prod_{p=1}^{j-1} f(d(x_j,x_p))^2 \quad \text{and} \quad F_i^2 \geq \prod_{p=1}^{i-1} f(d(x_i,x_p))^2.$$

Notice that, for any numbers $a_1, \ldots, a_m \in [0,1]$,

$$\prod_{p=1}^{m} a_p \geq 1 - \sum_{p=1}^{m} (1 - a_p). \tag{3.B.6}$$

Employing (3.B.6) in (3.B.5) we get

$$F_j^2 \cdots F_N^2 \geq \left(F_{j+1,j}^2 \cdots F_{i-1,j}^2\right)\left(F_{i+1,ij}^2 \cdots F_{N,ij}^2\right) A_j B_{ij}, \tag{3.B.7}$$

where

$$A_j := 1 - \sum_{p=1,p\neq i,j}^{N} \left(1 - f(d(x_p,x_j))^2\right) \quad \text{and} \quad B_{ij} := 1 - \sum_{p=1,p\neq i}^{N} \left(1 - f(d(x_p,x_i))^2\right).$$

We are now ready to estimate E_1. Since

$$F_i \leq f(d(x_i,x_j)) \quad \text{for } j < i \quad \text{and} \quad f'(t_i)^2 \leq \sum_{j=1}^{i-1} f'(d(x_i,x_j))^2,$$

we see that

$$E_1 \leq \sum_{i=2}^{N} \sum_{j=1}^{i-1} \frac{\int \left(2f'(d(x_i,x_j))^2 + f(d(x_i,x_j))^2 V(x_i - x_j)\right) (\Psi F_i^{-1})^2}{\int \Psi^2}. \tag{3.B.8}$$

By (3.B.4) and (3.B.7) we get

$$(\Psi F_i^{-1})^2 \leq \big(F_1^2 \cdots F_{j-1}^2\big) \cdot 1 \cdot \big(F_{j+1,j}^2 \cdots F_{i-1,j}^2\big)\big(F_{i+1,ij}^2 \cdots F_{N,ij}^2\big) \tag{3.B.9}$$

and

$$\Psi^2 \geq \big(F_1^2 \cdots F_{j-1}^2\big)\big(F_{j+1,j}^2 \cdots F_{i-1,j}^2\big)\big(F_{i+1,ij}^2 \cdots F_{N,ij}^2\big) A_i B_{ij}. \tag{3.B.10}$$

Employing (3.B.9) and (3.B.10) in (3.B.8) decouples the integration w.r.t. x_i and x_j and the rest of the integrals cancel out. Thus

$$E_1 \leq \sum_{i=2}^{N} \sum_{j=1}^{i-1} \frac{\int_{\Lambda^2} 2f'(d(x_i,x_j))^2 + V(x_i - x_j) f(d(x_i,x_j))^2 \, dx_i dx_j}{\int_{\Lambda^2} A_j B_{ij} \, dx_i dx_j}.$$

Since d is periodic with period L, we have

$$\int_\Lambda f'(d(x,y))^2 \, dx = \int_{y+\Lambda} f'(d(x,y))^2 \, dx = \int_{y+\Lambda} f'(|x-y|)^2 \, dx \leq \int_{\mathbb{R}^n} f'(|x|)^2 \, dx,$$

for each fixed $y \in \Lambda$. This observation, together with the fact that f is non-decreasing, yields

$$\int_\Lambda 2f'(d(x,y))^2 + V(x-y) f(d(x,y))^2 \, dx \leq \int_{\mathbb{R}^n} 2f'(|x|)^2 + V(x) f(|x|)^2 \, dx = J.$$

Also

$$\int_\Lambda B_{ij} \, dx_i = L^n - \sum_{p=1, p\neq i}^{N} \int_\Lambda \big(1 - f(d(x_i,x_p))^2\big) \, dx_i \geq L^n(1 - \rho I).$$

Similarly, the integral of A_j is bounded below by $L^n(1-\rho I)$. In total we have

$$E_1 \leq \sum_{i=2}^{N} \sum_{j=1}^{i-1} \frac{L^n J}{L^{2n}(1-\rho I)^2} \leq \frac{N}{2} \rho \frac{J}{(1-\rho I)^2}.$$

For the estimate of E_2 we employ (3.B.4) and obtain

$$\begin{aligned} \varepsilon_{ik}\varepsilon_{jk}(\Psi F_i^{-1})(\Psi F_j^{-1}) f'(t_i) f'(t_j) \quad &\leq \quad \big(F_1^2 \cdots F_{j-1}^2\big)\big[\varepsilon_{jk} f(t_j) f'(t_j)\big]\big(F_{j+1,j}^2 \cdots F_{i-1,j}^2\big) \\ &\times \quad \big[\varepsilon_{ik} f(t_i) f'(t_i)\big]\big(F_{i+1,ij}^2 \cdots F_{N,ij}^2\big), \end{aligned}$$

which together with (3.B.7) allows us to decouple integration w.r.t. x_j and x_i as in the estimate of E_1. Thus we have

$$E_2 \leq 2L^{-2n} \sum_{j<i} \sum_{k=1}^{j} \frac{\int_{\Lambda^2} \big[\varepsilon_{jk} f(t_j) f'(t_j)\big]\big[\varepsilon_{ik} f(t_i) f'(t_i)\big] \, dx_i dx_j}{(1-\rho I)^2}.$$

Since $\varepsilon_{ik} = 0$ except when $t_i = d(x_i, x_k)$ we have

$$\int_\Lambda \varepsilon_{ik} f(t_i) f'(t_i) \, dx_i \leq \int_\Lambda f(d(x_i,x_k)) f'(d(x_i,x_k)) \, dx_i \leq \int_{\mathbb{R}^n} f(|x|) f'(|x|) \, dx = K.$$

Next, the summation over k only contributes by a factor 2, since $\sum_{k=1}^{j}\varepsilon_{jk} = 2$ a.e. Since

$$\int_\Lambda f(t_i)f'(t_i)\,dx_i \le \sum_{p=1}^{j-1}\int_\Lambda f(d(x_p,x_i))f'(d(x_p,x_i))\,dx_i \le (j-1)K$$

we see that

$$E_2 \le 4L^{-2n}K^2\sum_{i=3}^{N}\sum_{j=2}^{i-1}(j-1) = \frac{2}{3}L^{-2n}K^2N(N-1)(N-2) \le \frac{2}{3}N\rho^2K^2.$$

By adding the contributions from E_1 and E_2 we arrive at the right-hand side in (3.B.1)
□

Chapter 4

The Second Order Upper Bound via Soft-Pair Fock States

In this chapter we consider a grand canonical version of the trial state introduced by Yau and Yin in [25], and we give an alternative and somewhat simpler proof of Theorem 1.3.3. We also consider the method in 4 dimensions, but with a negative outcome, in contrast to the calculations with the Bogoliubov trial state in Section 3.3. Our main result is the following upper bound, slightly stronger than the one of [25].

Theorem 4.0.2. *Let $n = 3$. Suppose that V is nonnegative, radially symmetric, smooth and compactly supported with $V(0) > 0$. Let $0 < \eta < 1/52$. Then*

$$e_0(\rho) \leq 4\pi a\rho\left(1 + \frac{128}{15\sqrt{\pi}} Y^{1/2}\right) + \mathcal{O}\big(\rho^{\frac{3}{2}+\eta}\big) \quad \textit{as } \rho \to 0.$$

The assumptions on V in Theorem 4.0.2 are presumably not optimal. In particular we expect the proof to work, assuming only finite smoothness and sufficiently fast decay at infinity. Furthermore, the error term can probably be improved, although we do not expect something even close to $\rho^2|\ln\rho|$ (i.e. the error term in Theorem 3.3.1) from the present approach.

The main idea of Yau and Yin was to extend the typical Bogoliubov trial state

$$\Psi^{\mathrm{Bog}} = \exp\left(\frac{1}{2}\sum_{p\neq 0} c_p a_p^+ a_{-p}^+ + \sqrt{N_0}a_0^+\right)|0\rangle \tag{4.0.1}$$

by allowing *soft-pair's*, i.e. particle pair's with momenta $q, p-q$, where $|p| \sim \rho^{1/2}$. This would (at least formally) be accomplished by a state of the form

$$\Psi = \exp\left(\frac{1}{\sqrt{N}}\sum_{\substack{p\neq 0\\ q\neq p,0}} \sqrt{c_q}\sqrt{c_{p-q}}a_q^+ a_{p-q}^+ a_p + \frac{1}{2}\sum_{p\neq 0} c_p a_p^+ a_{-p}^+ + \sqrt{N_0}a_0^+\right)|0\rangle.$$

This state turns out to be too complicated though (perhaps even to define properly), and instead a truncated version is constructed. Still, the truncated state is significantly more complicated to handle than the Bogoliubov state, due to the fact that more interaction terms contributes to the energy: Recall that the Bogoliubov state has the property that, if

$$\langle \Psi^{\mathrm{Bog}}, a_p^+ a_q^+ a_r a_s \Psi^{\mathrm{Bog}} \rangle \neq 0,$$

then either $p = -q$, $p = r$ or $p = s$. This does not hold true for the soft-pair state, and we get contributions from general quartets $a_p^+ a_q^+ a_r a_s$, where $p + q = r + s$. The most complicated case is when all four indices are nonzero. In particular, the energy estimates in this case are hardly compatible with the thermodynamic limit, and hence a detour is taken (Section 4.1 below). In [25] the soft-pair state is considered in a canonical ensemble with the particle number fixed. Our main observation is that some of the calculations become simpler in a grand canonical ensemble. The reason behind this is that, basically, the calculations with the trial state reduces to manipulations of (finite) sums in the canonical ensemble, and (infinite) series in the grand canonical ensemble. Due to the unbounded summation regime, the latter is often easier to handle.

We briefly fix notations. Suppose that $V \in C_0^\infty(\mathbb{R}^n)$, with $n \geq 3$, is nonnegative and radially symmetric with $V(0) > 0$. Let $1 - w$ denote the the zero-energy scattering solution and let a denote the scattering length. We reserve the notations

$$\varphi := Vw, \quad g := V - \varphi \quad \text{and} \quad \hat{w}_p := \frac{\hat{g}_p}{2p^2}.$$

Let $\mathcal{F}_L$ denote the bosonic Fock space over $L^2(\Lambda_L)$, and let H_L^{Dir} denote the second quantization of $H_{N,L}$ with Dirichlet boundary conditions. Recall the corresponding (Dirichlet) 'grand canonical ground state energy' $E_0^{\mathrm{GC}}(N, L)$ from (2.0.2) along with Lemma 2.0.1. Then let H_L^{per} denote the second quantization of $H_{N,L}$ with periodic boundary conditions *and* with V replaced by its L-periodization, given in (2.0.3). Finally, recall the representation

$$H_L^{\mathrm{per}} = \sum_p p^2 a_p^+ a_p + \frac{1}{2|\Lambda|} \sum_{\substack{p,q,r,s \\ p+q=r+s}} \hat{V}_{p-r} a_p^+ a_q^+ a_r a_s \tag{4.0.2}$$

in the sense of quadratic forms.

4.1 Reduction to Small Torus

In Section 4.2 we construct, for fixed ρ, L, a periodic Fock state $\Psi \in \mathcal{F}_L$ with expected number of particles

$$\rho L^n \leq \langle \mathcal{N} \rangle_\Psi \leq C \rho L^n.$$

The following lemma, which we prove in Appendix 4.A, shows that the energy in the periodic state almost yields an upper bound on the grand canonical (Dirichlet) ground state energy in a slightly larger box.

Lemma 4.1.1. *Let $L > 2l > 0$. Then*

$$E_0^{GC}(N, L + 2l) \leq \langle H_L^{per} \rangle_\Psi + C \frac{N}{lL},$$

for each periodic, normalized $\Psi \in \mathcal{F}_L$ with $N \leq \langle \mathcal{N} \rangle_\Psi \leq C'N$. Here $C, C' > 0$ depend only on n.

Our energy estimates in the trial state Ψ will only have the desired form if the side length of the box Λ_L does not exceed $\sim \rho^{-1}$, and in particular, we cannot take the limit $L \to \infty$, for fixed ρ. The next lemma is proved in Appendix 4.B and shows that we may still obtain an upper bound to the ground state energy in the thermodynamic limit, by 'sacrificing' density.

Lemma 4.1.2. *Suppose that* $supp(V) \subset B(0,R)$. *Let* $N, L, \rho > 0$ *with* $\rho = N/L^n$. *Then*

$$\frac{E_0^{GC}(N,L)}{N} \geq e_0\big(\rho[1+R/L]^{-n}\big),$$

We will prove the following theorem for the case $n = 3$:

Theorem 4.1.3. *Let* $\rho > 0$ *and* $L = \rho^{-\gamma}$, *where* $1 < \gamma < 1 + 1/52$. *There exists a periodic state* $\Psi \in \mathcal{F}_L$ *such that*

$$\frac{\langle H_L^{per}\rangle_\Psi}{\rho L^3} \leq 4\pi a\rho\left(1 + \frac{128}{15\sqrt{\pi}}Y^{1/2}\right) + C\rho^{1/2+\gamma}. \tag{4.1.1}$$

We obtain an upper bound on $e_0(\rho)$ from Theorem 4.1.3 as follows: Denote the right-hand side of (4.1.1) by $E(\rho)$. Let $l < L/2$ and put

$$\tilde{\rho} := \frac{\rho L^3}{(L+2l)^3},$$

so that $\rho L^3 = \tilde{\rho}(L+2l)^3$. Then the Lemma 4.1.2 above yields

$$\begin{aligned}\frac{E_0^{\mathrm{GC}}(\rho L^3, L+2l)}{\rho L^3} &= \frac{E_0^{\mathrm{GC}}(\tilde{\rho}(L+2l)^3, L+2l)}{\tilde{\rho}(L+2l)^3} \\ &\geq e_0\big(\tilde{\rho}[1+R/(L+2l)]^{-3}\big) \\ &= e_0\big(\rho[1+(2l+R)/L]^{-3}\big).\end{aligned}$$

Combining with Lemma 4.1.1 and Theorem 4.1.3, we have

$$e_0\big(\rho[1+(2l+R)/L]^{-3}\big) \leq E(\rho) + \frac{C}{lL},$$

and therefore also

$$e_0(\rho) \leq E\big(\rho[1+(2l+R)/L]^3\big) + \frac{C}{lL}.$$

We will take $l = L^\alpha$, for some $0 < \alpha < 1$. Using the fact that $\rho \mapsto E(\rho)$ is increasing, we arrive at

$$e_0(\rho) \leq E(\rho) + C\big[\rho^{1+\gamma(1-\alpha)} + \rho^{\gamma(1+\alpha)}\big].$$

For given γ, the optimal choice for α is $\alpha = 1/(2\gamma)$. With this choice we have

$$e_0(\rho) \leq E(\rho) + C\rho^{1/2+\gamma}.$$

This proves Theorem 4.0.2.

4.2 Construction of the Trial State

Fix $\rho, L > 0$. We define a trial state

$$\Psi := \sum_{\alpha} f(\alpha)|\alpha\rangle \tag{4.2.1}$$

in terms of the orthonormal basis $\{|\alpha\rangle\}_\alpha \subset \mathcal{F}_L$ given by

$$|\alpha\rangle := \prod_{k\in\Lambda^*} \frac{1}{\sqrt{\alpha(k)!}}(a_k^+)^{\alpha(k)}|0\rangle,$$

for each $\alpha : \Lambda^* \to \mathbb{N}_0$ with $|\alpha| := \sum_{k\in\Lambda^*} \alpha(k) < \infty$. From the CCR it follows that

$$a_p|\alpha\rangle = \sqrt{\alpha(p)}|\alpha - \delta_p\rangle \quad \text{and} \quad a_p^+|\alpha\rangle = \sqrt{\alpha(p)+1}|\alpha + \delta_p\rangle, \tag{4.2.2}$$

for any $p \in \Lambda^*$, where $\delta_p(k) := \delta_{p,k}$. Let

$$\mathcal{M} := \big\{\alpha : \Lambda^* \to \mathbb{N}_0 : \ |\alpha| < \infty, \ \alpha(-p) = \alpha(p) \text{ for each } p \in \Lambda^*\big\}.$$

For each $p \neq 0$ we define the *strict-pair* operation $\mathcal{A}^p$ by

$$\mathcal{A}^p\alpha(k) := \begin{cases} \alpha(k)+1 & k = \pm p \\ \alpha(k) & \text{otherwise} \end{cases}.$$

The inverse of $\mathcal{A}^p$ is denoted by $\mathcal{A}_p$. Notice that any $\alpha \in \mathcal{M}$ can be represented as

$$\alpha = \prod_{p\neq 0} \left(\mathcal{A}^p\right)^{\alpha(p)}\beta,$$

for some $\beta : \Lambda^* \to \mathbb{N}_0$ with $\beta(p) = 0$, for each $p \neq 0$. Given any $p, q \in \Lambda^*\backslash\{0\}$ with $p \neq q$ we define the *soft-pair* operation $\mathcal{A}^{p,q}$ by

$$\mathcal{A}^{p,q}\alpha(k) := \begin{cases} \alpha(k)-1 & k = p \\ \alpha(k)+1 & k = q, p-q \\ \alpha(k) & \text{otherwise} \end{cases},$$

with inverse $\mathcal{A}_{p,q}$. Suppose that

$$0 < 8\varepsilon_L < 4R_L \leq 2\varepsilon_H < R_H \tag{4.2.3}$$

and define the two subsets

$$P_L := \{p \in \Lambda^* : \varepsilon_L \leq |p| \leq R_L\}, \quad P_H := \{p \in \Lambda^* : \varepsilon_H \leq |p| \leq R_H\}.$$

We will eventually choose

$$\varepsilon_L = \rho^{1/2+\eta}, \quad R_L = \rho^{1/2-\eta}, \quad \varepsilon_H = \rho^{\eta}, \quad R_H = \rho^{-\eta}, \tag{4.2.4}$$

where $0 < \eta < 1/52$. However, we want to keep track of these parameters, and besides our calculation only uses (4.2.3). Now define M to be the union of $\mathcal{M}$ with the set of all *finite* derivations of the form $\prod_{j=1}^m \mathcal{A}^{p_j,q_j}\beta$, where $m \in \mathbb{N}$,

$$p_j \in P_L \text{ with } p_j \neq \pm p_k, \quad q_j, (p_j - q_j) \in P_H \quad \text{and } \beta \in \mathcal{M} \text{ with } \beta(p_j) \geq 1.$$

Note that the condition $p_j \neq \pm p_k$ implies that, for each $\alpha \in M$,

$$|\alpha(p) - \alpha(-p)| \leq 1, \quad \text{for each } p \in P_L.$$

We let

$$\alpha^*(p) := \max\{\alpha(p), \alpha(-p)\}.$$

Also define

$$M_p^s := \{\alpha \in M : \alpha(-p) = \alpha(p)\} \quad \text{and} \quad M_p^a := M \backslash M_p^s.$$

By construction, $M_p^s = M$, for $p \notin P_L \cup P_H$. Suppose that $c : \Lambda^* \backslash \{0\} \to (-1,1)$ has fast decay and satisfies $c_{-p} = c_p$, for each $p \neq 0$. Let

$$N_0 := N - \sum_{p \neq 0} \frac{c_p^2}{1 - c_p^2}, \tag{4.2.5}$$

where $N := \rho|\Lambda| = \rho L^n$. We define the coefficient function f in (4.2.1) by

$$f(\alpha) := C\left(\frac{N_0^{\alpha(0)}}{\alpha(0)!}\right)^{1/2} \prod_{k \neq 0} c_k^{\alpha(k)/2} \prod_{\substack{v \in P_L \\ \alpha^*(v) - \alpha(v) = 1}} \left(\frac{4\alpha^*(v) c_v}{N}\right)^{1/2},$$

for $\alpha \in M$ and $f(\alpha) = 0$ otherwise. Here $C > 0$ is a normalization constant and we use the convention $\sqrt{x} := i\sqrt{|x|}$ if $x < 0$. We warn the reader that, in general, $\sqrt{xy} \neq \sqrt{x}\sqrt{y}$. We also remark that f restricted to $\mathcal{M}$ yields the Bogoliubov state in (4.0.1). For the remaining part of this chapter we set

$$H := H_L^{\text{per}} \quad \text{and} \quad \langle A \rangle := \langle A \rangle_\Psi,$$

with Ψ given in (4.2.1).

4.3 The Pair-Hamiltonian

From the total Hamiltonian (4.0.2) we single out the kinetic energy and interaction terms where either $p = r, s, -q$. Thus we let

$$H_P := \sum_p p^2 a_p^+ a_p + H_{P1} + H_{P2} + H_{P3},$$

where

$$H_{P1} := \frac{\hat{V}_0}{2|\Lambda|} \sum_{p,q} a_p^+ a_q^+ a_p a_q, \quad H_{P2} := \frac{1}{2|\Lambda|} \sum_{p \neq q} \hat{V}_{p-q} a_p^+ a_q^+ a_p a_q$$

and

$$H_{P3} := \frac{1}{2|\Lambda|} \sum_{p \neq \pm q} \hat{V}_{p-q} a_p^+ a_{-p}^+ a_q a_{-q}.$$

Our first result in this section shows that, for momenta outside P_L and P_H, the expectations in H_P can be calculated directly in terms of the c_p's. The central observation is the relations

$$f(\alpha + \delta_0) = N_0^{1/2}(\alpha(0)+1)^{-1/2} f(\alpha) \quad \text{and} \quad f(\mathcal{A}^p \alpha) = c_p f(\alpha),$$

for $p \in P_H$ or $\alpha \in M_p^s$. Given any $p_1, \dots, p_n \in \Lambda^*$, we use the notation

$$Q(p_1, \dots, p_n) := \langle (a_{p_1}^+ a_{p_1}) \dots (a_{p_n}^+ a_{p_n}) \rangle = \sum_\alpha \alpha(p_1) \cdots \alpha(p_n) |f(\alpha)|^2.$$

We also introduce the functions

$$h_p := \frac{c_p^2}{1 - c_p^2} \quad \text{and} \quad s_p := \frac{c_p}{1 - c_p^2}.$$

Finally, it is convenient to have the notation

$$R_{p,q}^{r;s}(\alpha) := \sqrt{\alpha(p)\alpha(q)(\alpha(r)+1)(\alpha(s)+1)},$$

with the further convention that if one (or more) of the four indices on the LHS is omitted, the corresponding factor(s) on the RHS is replaced by one.

Lemma 4.3.1. *Suppose that $p, q, p_1, \dots, p_n \in \Lambda^*$ and $p \notin P_L \cup P_H$.*

(i) For any operator A on $\mathcal{F}$ (with domain containing Ψ and $a_0\Psi$) we have

$$\langle A a_0 \rangle = \sqrt{N_0} \langle A \rangle.$$

(ii) If $p \neq 0$ then

$$Q(p) = h_p, \quad \langle a_p^+ a_{-p}^+ \rangle = s_p = \langle a_p a_{-p} \rangle \quad \text{and} \quad Q(p, \pm p) = h_p(2h_p + 1).$$

(iii) If $p \neq \pm p_i$, for $i = 1, \dots, n$, then

$$Q(p, p_1, \dots, p_n) = Q(p) Q(p_1, \dots, p_n).$$

(iv) If $p \neq \pm q$, then

$$\langle a_q^+ a_{-q}^+ a_p a_{-p} \rangle = \langle a_q^+ a_{-q}^+ \rangle \langle a_p a_{-p} \rangle.$$

Proof. By definition of Ψ and the relation in (4.2.2),

$$\begin{aligned} \langle A a_0 \rangle &= \sum_{\alpha,\beta} \overline{f(\beta)} f(\alpha) \langle \beta | A a_0 | \alpha \rangle = \sum_{\alpha,\beta} \overline{f(\beta)} f(\alpha) \sqrt{\alpha(0)} \langle \beta | A | \alpha - \delta_0 \rangle \\ &= \sum_{\alpha,\beta} \overline{f(\beta)} f(\alpha + \delta_0) \sqrt{(\alpha + \delta_0)(0)} \langle \beta | A | \alpha \rangle = \sqrt{N_0} \langle A \rangle. \end{aligned}$$

In the third equality we have used the fact that $\{\alpha \in M : \alpha(0) \geq 1\} = \{\alpha+\delta_0 : \alpha \in M\}$. Next, since the symmetry $\alpha(-p) = \alpha(p)$ is preserved for p outside $P_L \cup P_H$, we have $\{\alpha \in M : \alpha(p) \geq 1\} = \{\mathcal{A}^p\alpha : \alpha \in M\}$, and hence

$$Q(p) = \sum_{\alpha} \alpha(p)|f(\alpha)|^2 = \sum_{\alpha}(\alpha(p)+1)|f(\mathcal{A}^p\alpha)|^2 = c_p^2(Q(p)+1).$$

Solving for $Q(p)$ yields $Q(p) = h_p$. The identity (iii) is proved completely similarly, since $\alpha(p_i)$ is not affected by $\mathcal{A}^p$. For a 'pair-operator' $a_p^+a_{-p}^+$ we have

$$\begin{aligned}\langle a_p^+a_{-p}^+\rangle &= \sum_{\alpha} \overline{f(A^p\alpha)}f(\alpha)R^{p,-p}(\alpha)\\ &= c_p\sum_{\alpha}|f(\alpha)|^2(\alpha(p)+1) = c_p(Q(p)+1)\\ &= c_p(h_p+1) = s_p.\end{aligned}$$

Then, for a double 'pair-operator',

$$\begin{aligned}\langle a_q^+a_{-q}^+a_pa_{-p}\rangle &= \sum_{\alpha} \overline{f(\mathcal{A}^q\mathcal{A}_p\alpha)}f(\alpha)R^{q,-q}(\alpha)\alpha(p)\\ &= c_p^2\sum_{\alpha} \overline{f(\mathcal{A}^q\mathcal{A}_p\alpha)}f(\alpha)R^{q,-q}(\alpha)(\alpha(p)+1)\\ &= c_p^2\Bigg(\langle a_q^+a_{-q}^+a_pa_{-p}\rangle + \sum_{\alpha}\overline{f(\mathcal{A}^q\mathcal{A}_p\alpha)}f(\alpha)R^{q,-q}(\alpha)\Bigg)\\ &= c_p^2\langle a_q^+a_{-q}^+a_pa_{-p}\rangle + c_p\langle a_q^+a_{-q}^+\rangle,\end{aligned}$$

and hence

$$\langle a_q^+a_{-q}^+a_pa_{-p}\rangle = s_p\langle a_q^+a_{-q}^+\rangle = \langle a_q^+a_{-q}^+\rangle\langle a_pa_{-p}\rangle.$$

Finally,

$$Q(p,\pm p) = c_p^2\sum_{\alpha}(\alpha(p)+1)(\alpha(\pm p)+1)|f(\alpha)|^2 = c_p^2\big(Q(p,\pm p)+2Q(p)+1\big),$$

where we have also used $Q(p) = h_p = Q(-p)$. It follows that $Q(p,\pm p) = h_p(2h_p+1)$ as desired. □

In order to calculate the energy of H_P it remains to obtain good estimates for the quantities in Lemma 4.3.1, for $p, q \in P_L \cup P_H$. This is done in Lemma 4.3.2, Lemma 4.3.4, Lemma 4.3.5 and Lemma 4.3.6 below. Notice the relations

$$f(\mathcal{A}^p\alpha) = c_p\sqrt{\frac{\alpha^*(p)+1}{\alpha^*(p)}}f(\alpha) \quad \text{if } p \in P_L \text{ and } \alpha \in M_p^a \tag{4.3.1}$$

$$f(\mathcal{A}^{p,q}\alpha) = \sqrt{c_q}\sqrt{c_{p-q}}\sqrt{\frac{4\alpha(p)}{N}}f(\alpha) \quad \text{if } p \in P_L \text{ and } \alpha \in M_p^s. \tag{4.3.2}$$

In Table 4.1 below we have listed various quantities, with which we express the (presumable) error terms in our further calculation. Most of them will not appear before Proposition 4.3.7, and some not before Section 4.4. Our motivation from the particular grouping of terms comes from the choice of c_p in [4] and the calculation in Section 3.3, where $c_p \approx 1$, for $p \in P_L$ and $c_p \approx -\rho\hat{w}_p$, for $p \in P_H$, assuming (4.2.4) also. Notice that, since $|c_p| < 1$, and by (4.2.5) we have $I \leq K \leq 1$. We introduce a new variable

$$e_p := \frac{c_p}{1+c_p}, \quad h_p = \frac{e_p^2}{1-2e_p}, \quad s_p = \frac{e_p(1-e_p)}{1-2e_p},$$

and we note that the constraint $|c_p| < 1$ is equivalent to $e_p < 1/2$. Furthermore, let

$$\tilde{h}_p := (1+h_p)\Bigg(1 - \frac{4|s_p|}{N} \sum_{\substack{v \in P_L \\ v-p \in P_H}} |c_{v-p}| h_v\Bigg)^{-1} \frac{4|s_p|}{N} \sum_{\substack{v \in P_L \\ v-p \in P_H}} |c_{v-p}| h_v.$$

Finally we set

$$\delta := \sup_{p \in P_H} |c_p| \quad \text{and} \quad s_c := 1 + \sup_{p \in P_L} |s_p| \quad \text{and} \quad h_c := 1 + \sup_{p \in P_L} h_p.$$

Note that $h_p \leq |s_p|$ always, and hence in particular $h_c \leq s_c$. We further assume that

$$I h_c^2 \leq 1 \quad \text{and} \quad \delta < 1/2. \tag{4.3.3}$$

In particular, the latter assumption implies that

$$\tilde{h}_p = \mathcal{O}(K\delta s_p), \quad \text{for } p \in P_H. \tag{4.3.4}$$

$\times N$		$\times N$		$\times N$	
I	$\sum_{p \in P_H} c_p^2$	J	$\sum_{p \neq 0} \lvert s_p \rvert$	K	$\sum_{p \neq 0} h_p$
$\tilde{I}$	$\sum_{p \neq 0} \lvert c_p \rvert^{1/2}$	$\tilde{J}$	$\sum_{p \neq 0} s_p^2$	$\tilde{K}$	$\sum_{p \neq 0} h_p^2$
S	$\sum_{p \neq 0} \lvert p \rvert h_p$	T	$\sum_{p \neq 0} p^2 h_p$	U	$\sum_{p \neq 0} \lvert e_p \rvert$
W	$\sum_{p \neq 0} \lvert e_p + \rho\hat{w}_p \rvert$	J_0	$\sum_{p \in P_L} \lvert s_p \rvert$	K_0	$\sum_{p \in P_L} h_p$
I_1	$\sum_{p \neq 0} \lvert c_p \rvert$	W_1	$\lvert c_p + \rho\hat{w}_p \rvert$		

Table 4.1: Various quantities appearing in the error terms. The notation here means that $I = N^{-1} \sum_{p \in P_H} c_p^2$ and so on.

Lemma 4.3.2. *We have*

$$h_p \leq Q(p) \leq \begin{cases} h_p(1 + CIh_c) \leq Ch_p, & p \in P_L \\ h_p + \tilde{h}_p \leq C\delta|s_p|, & p \in P_H. \end{cases}$$

Proof. Notice that $\mathcal{A}^p(M) \subseteq M$ for each $p \neq 0$. Then

$$Q(p) \geq \sum_{\alpha \in \mathcal{A}^p(M)} \alpha(p)|f(\alpha)|^2 = \sum_{\beta \in M} \mathcal{A}^p\beta(p)|f(\mathcal{A}^p\beta)|^2 \geq c_p^2(Q(p)+1),$$

where the second inequality comes from the case where $p \in P_L$ and $\beta \in M_p^a$. It follows that $Q(p) \geq h_p$. For the upper bounds, we suppose first that $p \in P_L$. Write

$$Q(p) = \sum_{\alpha \in M_p^s} \alpha(p)|f(\alpha)|^2 + \sum_{\alpha \in M_p^a} \alpha(p)|f(\alpha)|^2 =: Q^s(p) + Q^a(p).$$

Following the argument in the proof of Lemma 4.3.1 (ii) we see that

$$Q^s(p) = h_p \sum_{\alpha \in M_p^s} |f(\alpha)|^2 \leq h_p.$$

To estimate $Q^a(p)$ we notice that M_p^a is generated from M_p^s via soft-pair operations. That is, for each $\alpha \in M_p^a$ with, say, $\alpha^*(p) = \alpha(-p)$, there exist $q \in P_H$ with $p - q \in P_H$ and $\beta \in M_p^s$ with $\beta(p) \geq 1$, such that $\alpha = \mathcal{A}^{p,q}\beta$. Thus we have the upper bound

$$\begin{aligned}\sum_{\substack{\alpha \in M_p^a \\ \alpha^*(p)=\alpha(-p)}} \alpha(p)|f(\alpha)|^2 &\leq \sum_{\beta \in M_p^s} \sum_{\substack{q \in P_H \\ p-q \in P_H}} \mathcal{A}^{p,q}\beta(p)|f(\mathcal{A}^{p,q}\beta)(p)|^2 \qquad (4.3.5)\\ &= \sum_{\beta \in M_p^s} \sum_{\substack{q \in P_H \\ p-q \in P_H}} (\beta(p)-1)\beta(p)\frac{4}{N}|c_q| \cdot |c_{p-q}||f(\beta)|^2 \\ &\leq 4I \sum_{\beta \in M_p^s} (\beta(p)-1)\beta(p)|f(\beta)|^2,\end{aligned}$$

where the equality follows from the relation (4.3.2), and where we have used the Cauchy-Schwarz in the last estimate. Again, by following the strategy used in the proof of Lemma 4.3.1, we obtain

$$\sum_{\beta \in M_p^s} (\beta(p)-1)\beta(p)|f(\beta)|^2 = 2h_p \sum_{\beta \in M_p^s} \beta(p)|f(\beta)|^2 = 2h_p^2 \sum_{\beta \in M_p^s} |f(\beta)|^2 \leq 2h_p^2.$$

It follows that the left-hand side in (4.3.5) is bounded by $8Ih_p^2$. Similarly we bound the sum where $\alpha^*(p) = \alpha(p)$, but the contribution from this case is $4Ih_p(2h_p+1)$. Using the bound $h_p + 1 \leq h_c$ we obtain the desired.

Now suppose that $p \in P_H$ and write

$$Q(p) = \sum_{\alpha \in \mathcal{A}^p(M)} \alpha(p)|f(\alpha)|^2 + \sum_{\alpha \in M \setminus \mathcal{A}^p(M)} \alpha(p)|f(\alpha)|^2 =: A + B.$$

Clearly

$$A = \sum_{\beta \in M} \mathcal{A}^p\beta(p)|f(\mathcal{A}^p\beta)|^2 = c_p^2(Q(p)+1), \qquad (4.3.6)$$

and hence

$$Q(p) = h_p + (1 + h_p)B. \tag{4.3.7}$$

If $\alpha \in M \backslash \mathcal{A}^p(M)$ with $\alpha(p) \geq 1$, then there exist a $v \in P_L$ with $v - p \in P_H$ and a $\beta \in M_v^s$ such that $\mathcal{A}^{v,p}\beta = \alpha$. Thus B may be bounded as

$$\begin{aligned} B &\leq \sum_{\substack{v \in P_L \\ v-p \in P_H}} \sum_{\beta \in M_v^s} \mathcal{A}^{v,p}\beta(p) |f(\mathcal{A}^{v,p}\beta)|^2 \\ &= 4N^{-1} \sum_{\substack{v \in P_L \\ v-p \in P_H}} |c_p||c_{v-p}| \sum_{\beta \in M_v^s} \beta(v)(\beta(p)+1)|f(\beta)|^2 \\ &\leq 4N^{-1}|c_p|(Q(p)+1) \sum_{\substack{v \in P_L \\ v-p \in P_L}} |c_{v-p}| h_v \\ &= 4N^{-1} \frac{|c_p|}{1-c_p^2}(B+1) \sum_{\substack{v \in P_L \\ v-p \in P_H}} |c_{v-p}| h_v, \end{aligned}$$

and it follows that $B \leq \tilde{h}_p/(1+h_p)$. Together with (4.3.7), this shows the upper bound in case $p \in P_H$. □

Remark 4.3.3. *From Lemma 4.3.1, Lemma 4.3.2 and* (4.2.5) *it follows that*

$$N \leq \langle \mathcal{N} \rangle \leq N\big[1 + CK(Ih_c + \delta J)\big].$$

The estimates in the following lemma can be obtained using the strategy of Lemma 4.3.2 and the assumptions in (4.3.3), so we skip the proof. We say that vectors $p_1, \dots, p_m$ are $\pm$ *different* if $p_i \neq \pm p_j$, for each $i \neq j$.

Lemma 4.3.4. *(i) If $p_1, \dots, p_n \in P_L$ are $\pm$ different, then*

$$Q(p_1, \dots, p_n) \leq C h_{p_1} Q(p_2, \dots, p_n).$$

(ii) If $q_1, \dots, q_m \in P_H$ are $\pm$ different and $p_1, \dots, p_n \notin P_H$, then

$$Q(p_1, \dots, p_n, q_1, \dots, q_m) \leq C_m \delta^m |c_{q_1} \cdots c_{q_m}| Q(p_1, \dots, p_n)$$

(iii) For $p \neq 0$,

$$Q(p, \pm p) \leq C \cdot \begin{cases} h_c h_p, & p \in P_L \\ \delta |s_p|, & p \in P_H \end{cases}.$$

Lemma 4.3.5. *We have*

$$\langle a_p^+ a_{-p}^+ \rangle = \begin{cases} s_p\big[1 + \mathcal{O}(Ih_c)\big] & \text{if } p \in P_L \\ s_p\big[1 + \mathcal{O}(\delta |c_p|)\big] & \text{if } p \in P_H \end{cases}.$$

Proof. For any $p \neq 0$ we have

$$\langle a_p^+ a_{-p}^+ \rangle = \sum_\alpha \overline{f(\mathcal{A}^p \alpha)} f(\alpha) R^{p,-p}(\alpha).$$

For $p \in P_L$ we write $\langle a_p^+ a_{-p}^+ \rangle = A + B$, where

$$\begin{aligned} A := \sum_{\alpha \in M_p^s} \overline{f(\mathcal{A}^p \alpha)} f(\alpha) R^{p,-p}(\alpha) &= c_p \sum_{\alpha \in M_p^s} |f(\alpha)|^2 (\alpha(p) + 1) \\ &= c_p (h_p + 1) \sum_{\alpha \in M_p^s} |f(\alpha)|^2 = s_p - s_p \sum_{\alpha \in M_p^a} |f(\alpha)|^2. \end{aligned}$$

From (4.3.1) we get

$$B = c_p \sum_{\alpha \in M_p^a} |f(\alpha)|^2 (\alpha^*(p) + 1).$$

Following the proof of Lemma 4.3.2 we use the fact that M_p^a is generated from M_p^s via soft-pair operations to obtain

$$\sum_{\alpha \in M_p^a} |f(\alpha)|^2 \leq 8 I h_p \quad \text{and} \quad \sum_{\alpha \in M_p^a} |f(\alpha)|^2 \alpha^*(p) \leq 8 I h_p (2 h_p + 1). \tag{4.3.8}$$

The result now follows, since $h_p + 1 \leq h_c$ and $h_p \leq |s_p|$.

For $p \in P_H$ we have

$$\langle a_p^+ a_{-p}^+ \rangle = c_p \sum_\alpha |f(\alpha)|^2 R^{p,-p}(\alpha) = c_p + c_p \sum_\alpha |f(\alpha)|^2 \big(R^{p,-p}(\alpha) - 1 \big),$$

and the result follows from the inequality

$$0 \leq \left(\sqrt{(a+1)(b+1)} - 1 \right) \leq \frac{1}{2}(a+b), \quad a, b \geq 0, \tag{4.3.9}$$

Lemma 4.3.2 and the identity $c_p = s_p(1 - c_p^2)$. □

Lemma 4.3.6. *For $p \neq \pm q$ we have*

$$\langle a_p^+ a_{-p}^+ a_q a_{-q} \rangle = \begin{cases} s_p s_q \big[1 + \mathcal{O}(I h_c) \big] & p, q \in P_L \\ s_p s_q \big[1 + \mathcal{O}\big(\delta |s_p| + I h_c \big) \big] & p \in P_H, q \in P_L \\ s_p s_q \big[1 + \mathcal{O}\big(\delta (|s_p| + |s_q|) \big) \big] & p, q \in P_H \end{cases}.$$

Proof. For any $p, q \in \Lambda^*$ with $p \neq \pm q$ we have

$$\langle a_p^+ a_{-p}^+ a_q a_{-q} \rangle = \sum_\alpha \overline{f(\mathcal{A}^p \mathcal{A}_q \alpha)} f(\alpha) R_{q,-q}^{p,-p}(\alpha). \tag{4.3.10}$$

Suppose first that $q \in P_L$. In analogue to the proof of Lemma 4.3.5 we split the sum in (4.3.10) into a part over M_q^s (denoted A) and a part over M_q^a (denoted B). By following the calculation in the proof of Lemma 4.3.1 (iv) we obtain

$$A = s_q \langle a_p^+ a_{-p}^+ \rangle - s_q \sum_{\alpha \in M_q^a} \overline{f(\mathcal{A}^p \alpha)} f(\alpha) R^{p,-p}(\alpha).$$

Hence

$$
\begin{aligned}
|A - s_q\langle a_p^+ a_{-p}^+\rangle| &\le |s_q c_p| \sum_{\alpha\in M_q^a} |f(\alpha)|^2(\alpha^*(p)+1) \\
&\le 8I|s_q c_p| \sum_{\alpha\in M_q^s} |f(\alpha)|^2 \alpha(q)(\alpha^*(p)+1) \\
&\le 16 I h_q |s_q c_p|(Q(p)+1) \le C I h_q |s_p s_q|. \qquad (4.3.11)
\end{aligned}
$$

For the term B we notice that, if $\alpha(q)$ and $\alpha(-q)$ are both positive, then $\alpha \in \mathcal{A}^q(M)$. It follows that

$$
|B| \le |c_p c_q| \sum_{\beta\in M_q^a} |f(\beta)|^2(\beta^*(p)+1)(\beta^*(q)+1),
$$

and using the fact that M_q^a is generated from M_q^s via soft-pair operations, we can show that B is also bounded by the the last expression in (4.3.11). The two first claims of the lemma then follows from the triangle inequality together with Lemma 4.3.5 and the relation $c_p = s_p(1-c_p^2)$. For $p, q \in P_H$ we write

$$
\begin{aligned}
\langle a_p^+ a_{-p}^+ a_q a_{-q}\rangle &= c_p \sum_\alpha \overline{f(\mathcal{A}_q\alpha)} f(\alpha) R_{q,-q}^{p,-p}(\alpha) \\
&= c_p \sum_\alpha \overline{f(\mathcal{A}_q\alpha)} f(\alpha) R_{q,-q}(\alpha) + \Omega \\
&= c_p\langle a_q a_{-q}\rangle + \Omega,
\end{aligned}
$$

where

$$
\begin{aligned}
\Omega &:= c_p \sum_\alpha \overline{f(\mathcal{A}_q\alpha)} f(\alpha) R_{q,-q}(\alpha)\big(R^{p,-p}(\alpha)-1\big) \\
&= c_p c_q \sum_\alpha |f(\alpha)|^2 R^{q,-q}(\alpha)\big(R^{p,-p}(\alpha)-1\big)
\end{aligned}
$$

satisfies

$$
|\Omega| \le \frac{1}{2}|c_p c_q| \sum_\alpha |f(\alpha)|^2(\alpha^*(q)+1)(\alpha(p)+\alpha(-p)) \le C\delta h_p |c_q|.
$$

Again the result follows from Lemma 4.3.5 and the identity $c_p = s_p(1-c_p^2)$. □

Recall that for any continuous function $F \in L^1(\mathbb{R}^n)$, decaying faster than $|p|^{-n-\varepsilon}$ at infinity, for some $\varepsilon > 0$, we have the convergence

$$
\lim_{L\to\infty} \frac{1}{L^n} \sum_{p\in\Lambda^*} F(p) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} F(p)\,dp. \qquad (4.3.12)
$$

Since we do not take the thermodynamic limit we will get L-dependent errors in our estimates. In this regard we employ the bound

$$
\big|\hat{w}_{p+v} - \hat{w}_p\big| \le C|v|\big(|p|^{-2} + |p|^{-3}\big),
$$

which holds for each $p, v \in \mathbb{R}^n$ with $|v|/|p| \le c < 1$. This follows from the Lipschitz continuity of $\hat{g}$ and the fact that $|\hat{g}_p| \le \hat{g}_0$. The relevant sums-to-integral error terms then turn out to be $\mathcal{E}_3(L) = L^{-1}\ln L$ and $\mathcal{E}_n(L) = L^{-1}$, if $n \ge 4$.

Proposition 4.3.7. *We have*

$$\frac{\langle H_P\rangle}{N} \le E^{Bog} + \frac{2\rho}{N}\sum_{p\neq 0}\hat{\varphi}_p h_p + \frac{1}{N}\sum_{p\in P_H} p^2\tilde{h}_p + \Omega_P, \tag{4.3.13}$$

where

$$E^{Bog} := \frac{\hat{g}_0}{2}\rho + \frac{1}{N}\sum_{p\neq 0} p^2\left[\frac{e_p^2 + 2\rho\hat{w}_p e_p}{1-2e_p} + (\rho\hat{w}_p)^2\right] \tag{4.3.14}$$

and

$$\Omega_P = C\rho\Big\{K(K+\delta J + Is_c) + J^2 s_c(\delta + I) + JS + \rho^{-1}IT + N^{-1}(\tilde{J} + \delta J + s_c K) + W^2 + U\mathcal{E}_n(L)\Big\}.$$

Remark 4.3.8. *By comparing with Lemma 3.3.6 and ignoring the Ω-terms, we see that the only new term in the energy of the pair-Hamiltonian is $N^{-1}\sum_{p\in P_H} p^2\tilde{h}_p$, corresponding to some extra kinetic energy (see the proof below).*

Proof. By Lemma 4.3.1 and Lemma 4.3.2 we have the following upper bound on the kinetic energy:

$$\sum_p p^2\langle a_p^+ a_p\rangle \le \sum_p p^2 h_p + \sum_{p\in P_H} p^2\tilde{h}_p + I\sum_{p\in P_L} p^2 h_p.$$

Using the CCR, Lemma 4.3.1 (i), (4.2.5) and the fact that $Q(p) \ge h_p \ge 0$ (Lemma 4.3.2) we have

$$\begin{aligned}
\langle H_{P1}\rangle &= \frac{\hat{V}_0}{2|\Lambda|}\left(\sum_{p,q} Q(p,q) - \sum_p Q(p)\right)\\
&= \frac{\hat{V}_0}{2|\Lambda|}\left(N_0(N_0+1) + 2N_0\sum_{p\neq 0} Q(p) + \sum_{p,q\neq 0} Q(p,q) - \sum_{p\neq 0} Q(p) - N_0\right)\\
&\le \frac{\hat{V}_0}{2|\Lambda|}\left(N^2 + 2N\sum_{p\neq 0}(Q(p) - h_p) + \sum_{p,q\neq 0} Q(p,q)\right).
\end{aligned}$$

Similarly,

$$\langle H_{P2}\rangle = \sum_{p\neq 0}\rho\hat{V}_p Q(p) - \left(\frac{1}{|\Lambda|}\sum_{p\neq 0}\hat{V}_p Q(p)\right)\sum_{p\neq 0} h_p + \frac{1}{2|\Lambda|}\sum_{\substack{p,q\neq 0\\ p\neq q}}\hat{V}_{p-q}Q(p,q)$$

and

$$\begin{aligned}\langle H_{P3}\rangle &= \sum_{p\neq 0}\rho\hat{V}_p\langle a_p^+a_{-p}^+\rangle - \left(\frac{1}{|\Lambda|}\sum_{p\neq 0}\hat{V}_p\langle a_p^+a_{-p}^+\rangle\right)\sum_{p\neq 0}h_p \\ &\quad + \frac{1}{2|\Lambda|}\sum_{\substack{p,q\neq 0\\ p\neq \pm q}}\hat{V}_{p-q}\langle a_p^+a_{-p}^+a_q a_{-q}\rangle\end{aligned}$$

By Lemma 4.3.1, Lemma 4.3.2 and Lemma 4.3.4 we have

$$\frac{1}{N}\sum_{p\neq 0}Q(p) = \mathcal{O}\big[K(1+\delta J)\big]$$

and

$$\frac{1}{N^2}\sum_{p,q\neq 0}Q(p,q) = \mathcal{O}\big[K^2+\delta JK+\delta^2J^2+N^{-1}(h_cK+\delta J)\big].$$

The last term $N^{-1}(h_cK+\delta J)$ arises from the special cases $p=\pm q$, and we have also used $|c_p|\leq|s_p|$. It follows that

$$\begin{aligned}\frac{\langle H_{P1}\rangle+\langle H_{P2}\rangle}{N} &\leq \frac{\hat{V}_0}{2}\rho + \frac{1}{|\Lambda|}\sum_{p\neq 0}\hat{V}_p h_p \\ &\quad + C\rho\big[K^2+\delta JK+IKh_c+\delta^2J^2+N^{-1}(h_cK+\delta J)\big].\end{aligned}$$

For H_{P3} we employ Lemma 4.3.5 and Lemma 4.3.6 to estimate

$$\begin{aligned}\frac{\langle H_{P3}\rangle}{N} &= \frac{1}{|\Lambda|}\sum_{p\neq 0}\hat{V}_p s_p + \frac{1}{2\rho|\Lambda|^2}\sum_{p,q\neq 0}\big(\hat{V}_{p-q}s_ps_q - 2\hat{V}_ps_ph_q\big) \\ &\quad + \mathcal{O}\Big\{\rho\big[(I+\delta)J^2s_c+\delta JK+N^{-1}\tilde{J}\big]\Big\}.\end{aligned}$$

From the relation $e_p = s_p - h_p$ we have

$$\sum_{p,q\neq 0}\big(\hat{V}_{p-q}s_ps_q-2\hat{V}_ps_ph_q\big) = \sum_{p,q\neq 0}\hat{V}_{p-q}(e_pe_q-h_ph_q)+2(\hat{V}_{p-q}-\hat{V}_p)s_ph_q,$$

so from the Lipschitz continuity of $\hat{V}$ we obtain

$$\frac{\rho}{2N^2}\sum_{p,q\neq 0}\big(\hat{V}_{p-q}s_ps_q-2\hat{V}_ps_ph_q\big) = \frac{\rho}{2N^2}\sum_{p,q\neq 0}\hat{V}_{p-q}e_pe_q + \mathcal{O}(\rho(K^2+JS)).$$

Now notice that

$$\begin{aligned}\frac{\rho}{2N^2}\sum_{p,q\neq 0}\hat{V}_{p-q}e_pe_q &= \frac{\rho}{2N^2}\sum_{p,q\neq 0}\hat{V}_{p-q}(e_p+\rho\hat{w}_p)(e_q+\rho\hat{w}_q) \\ &\quad - \frac{\rho^2}{N^2}\sum_{p,q\neq 0}\hat{V}_{p-q}\hat{w}_qe_p - \frac{\rho^3}{N^2}\sum_{p,q\neq 0}\hat{V}_{p-q}\hat{w}_q\hat{w}_p.\end{aligned}$$

Moreover, since $(2\pi)^n\hat{\varphi} = \hat{V} * \hat{w}$ and $V = g + \varphi$, we get

$$\frac{\hat{V}}{2}\rho = \frac{\hat{g}}{2}\rho + \frac{\rho}{2(2\pi)^n}\int \hat{V}_p\hat{w}_p\,dp = \frac{\hat{g}}{2}\rho + \frac{\rho}{2(2\pi)^n}\int \hat{g}_p\hat{w}_p\,dp + \frac{\rho}{2(2\pi)^n}\int \hat{\varphi}_p\hat{w}_p\,dp.$$

Finally, by adding up terms and by noting that

$$\frac{1}{|\Lambda|}\sum_{p\neq 0}\hat{V}_{p-q}\hat{w}_q = \frac{1}{(2\pi)^2}\int \hat{V}_{p-q}\hat{w}_q\,dq + \mathcal{O}(\mathcal{E}_n(L)),$$

the result follows. □

4.4 The Anti-Symmetric Interaction Terms

In this section we estimate the energy of the remaining part of the Hamiltonian,

$$H_A := H - H_P,$$

i.e. the interaction terms from (4.0.2) where $p \neq r, s, -q$. From H_A we further single out terms with (exactly) one zero-momentum operator. Thus we write $H_A = H_{A1} + H_{A2}$, where

$$\langle H_{A1}\rangle = \frac{2}{|\Lambda|}\sum_{\substack{p+q=r\\ p\neq r,-q,0}} \hat{V}_q \cdot \mathrm{Re}\,\langle a_p^+ a_q^+ a_r a_0\rangle. \tag{4.4.1}$$

4.4.1 Interaction with Three Non-zero Momenta

We start by noting that in (4.4.1) only terms with $p, q, r \in P_L \cup P_H$ give nonzero contribution, due to the fact that $\alpha(-p) = \alpha(p)$, for each $\alpha \in M$ and $p \notin P_L \cup P_H$. Moreover, by construction, for any $\alpha \in M$, $\sum_{k\in P_H}\alpha(k)$ is an even number, and hence we can assume that either none, or exactly two of the momenta p, q, r are contained in P_H. Thus, the only relevant expectations are the ones considered in the following lemma.

Lemma 4.4.1. *Suppose that p, q, r are $\pm$ different with $p + q = r$.*

(i) For $p, q \in P_H$ and $r \in P_L$,

$$\langle a_p^+ a_q^+ a_r a_0\rangle = 2\sqrt{N_0/N}\sqrt{c_p}\sqrt{c_q}h_r\left[1 + \mathcal{O}\big(Ih_r + \delta^2|c_r|^{-1}\big)\right].$$

(ii) For $q \in P_L$ and $p, r \in P_H$,

$$\langle a_p^+ a_q^+ a_r a_0\rangle = \mathcal{O}\big(\delta|c_pc_r|^{1/2}|s_q|\big).$$

(iii) For $p, q, r \in P_L$,

$$\langle a_p^+ a_q^+ a_r a_0\rangle = \mathcal{O}\big((I + N^{-1})|s_ps_qs_r|\big).$$

Proof. By Lemma 4.3.1 we have

$$\langle a_p^+ a_q^+ a_r a_0 \rangle = \sqrt{N_0} \sum_{\alpha} \overline{f(\mathcal{A}^{r,p}\alpha)} f(\alpha) R_r^{p,q}(\alpha). \tag{4.4.2}$$

Suppose first that $p, q \in P_H$ and $r \in P_L$. We split the sum in (4.4.2) into two parts A and B depending on whether $\alpha \in M_r^s$ respectively $\alpha \in M_r^a$.

$$\begin{aligned} A &:= \sqrt{N_0} \sum_{\alpha \in M_r^s} \overline{f(\mathcal{A}^{r,p}\alpha)} f(\alpha) R_r^{p,q}(\alpha) \\ &= 2\sqrt{N_0/N}\sqrt{c_p}\sqrt{c_q} \sum_{\alpha \in M_r^s} |f(\alpha)|^2 \alpha(r) R^{p,q}(\alpha) \\ &= 2\sqrt{N_0/N}\sqrt{c_p}\sqrt{c_q} h_r \sum_{\alpha \in M_r^s} |f(\alpha)|^2 R^{p,q}(\alpha) \\ &= 2\sqrt{N_0/N}\sqrt{c_p}\sqrt{c_q} h_r \Big[1 + \mathcal{O}\big(I h_r + \delta(|s_p| + |s_q|)\big) \Big], \end{aligned}$$

where we in the estimate have used (4.3.9), Lemma 4.3.2 and the first bound in (4.3.8). For the sum over M_r^a we note that

$$\{\alpha \in M_r^a : \mathcal{A}^{r,p}\alpha \in M\} = \mathcal{A}_{r,p}(M_r^s) \cap M, \tag{4.4.3}$$

where $\mathcal{A}_{r,p} := (\mathcal{A}^{r,p})^{-1}$ with

$$f(\mathcal{A}_{r,p}\alpha) = \frac{c_r}{\sqrt{c_p}\sqrt{c_q}} \sqrt{\frac{4(\alpha(r)+1)}{N}} f(\alpha), \quad \text{for } \alpha \in M_r^s.$$

Thus

$$\begin{aligned} B &= \sqrt{N_0} \sum_{\alpha \in M_r^s} \overline{f(\alpha)} f(\mathcal{A}_{r,p}\alpha) R_{p,q}^r(\alpha) \\ &= 2\sqrt{N_0/N} c_r c_p^{-1/2} c_q^{-1/2} \sum_{\alpha \in M_r^s} |f(\alpha)|^2 (\alpha(r)+1) R_{p,q}(\alpha) \\ &= 2\sqrt{N_0/N} s_r c_p^{-1/2} c_q^{-1/2} \sum_{\alpha \in M_r^s} |f(\alpha)|^2 R_{p,q}(\alpha), \end{aligned}$$

where we have also used $s_r = c_r(h_r + 1)$ in the last equality. From Lemma 4.3.2 and $1/(1 - c_p^2) \leq C$, for $p \in P_H$, we see that

$$B = \mathcal{O}\big[\sqrt{N_0/N}\sqrt{c_p}\sqrt{c_q} h_r \delta^2 c_r^{-1}\big].$$

Upon adding A and B and using $|s_p| + |s_q| \leq C\delta$ and $1 < |c_r|^{-1}$, we arrive at (i).

The case where $q \in P_L$ and $p, r \in P_H$ is similar: The sum in (4.4.2) is now splitted in parts over M_q^s and M_q^a. For $\alpha \in M_q^s$ and $\mathcal{A}^{r,p}\alpha \in M$ we then have relation

$$f(\mathcal{A}^{r,p}\alpha) = \frac{2c_q\sqrt{c_p}}{\sqrt{c_r}} \sqrt{\frac{\alpha(q)+1}{N}} f(\alpha).$$

For the sum over M_q^a we note that (4.4.3) still holds with M_r^s and M_r^a replaced by M_q^s respectively M_q^a and that, for $\alpha \in M_q^s$ with $\mathcal{A}_{r,p}\alpha \in M$ we have

$$f(\mathcal{A}_{r,p}\alpha) = \frac{2\sqrt{c_r}}{\sqrt{c_p}}\sqrt{\frac{\alpha(q)}{N}}f(\alpha).$$

Finally, we need to consider the case where $p, q, r \in P_L$. Once again the procedure is similar, except there are more cases to consider due to the three P_L momenta. We decompose M into 8 regimes:

$$\begin{aligned}
&M_1 = M_p^s \cap M_q^s \cap M_r^s, \quad M_2 = M_p^s \cap M_q^s \cap M_r^a, \quad M_3 = M_p^s \cap M_q^a \cap M_r^s,\\
&M_4 = M_p^s \cap M_q^a \cap M_r^a, \quad M_5 = M_p^a \cap M_q^s \cap M_r^s, \quad M_6 = M_p^a \cap M_q^s \cap M_r^a,\\
&M_7 = M_p^a \cap M_q^a \cap M_r^s, \quad M_8 = M_p^a \cap M_q^a \cap M_r^a.
\end{aligned}$$

As in the previous cases we use the fact that $\mathcal{A}^{r,p}$ reflects symmetry to have

$$\sum_{(M_4,M_6,M_7,M_8)} \overline{f(\mathcal{A}^{r,p}\alpha)}f(\alpha)R_r^{p,q} = \sum_{(M_5,M_3,M_2,M_1)} \overline{f(\alpha)}f(\mathcal{A}_{r,p}\alpha)R_{p,q}^r.$$

From the definition of f we now read of the following relations:

	$\overline{f(\mathcal{A}^{r,p}\alpha)}f(\alpha)R_r^{p,q}\lvert f(\alpha)\rvert^{-2}$	$\overline{f(\alpha)}f(\mathcal{A}_{r,p}\alpha)R_{p,q}^r\lvert f(\alpha)\rvert^{-2}$
M_1	$8N^{-3/2}c_pc_q[R_r^{p,q}(\alpha)]^2$	$8N^{-3/2}c_r[R_{p,q}^r(\alpha)]^2$
M_2	$2N^{-1/2}c_pc_qc_r^{-1}[R^{p,q}(\alpha)]^2$	$2N^{-1/2}[R_{p,q}(\alpha)]^2$
M_3	$2N^{-1/2}c_p[R_r^p(\alpha)]^2$	$2N^{-1/2}c_q^{-1}c_r[R_p^r(\alpha)]^2$
M_5	$2N^{-1/2}c_q[R_r^q(\alpha)]^2$	$2N^{-1/2}c_p^{-1}c_r[R_q^r(\alpha)]^2$

The result then easily follows from a direct calculation together with the estimates (4.3.9), $N_0 \leq N$ and $|c_k| \leq 1$. □

Remark 4.4.2. *The above analysis may of course also be carried out in either of the special cases $p = q$, $p = -r$ or $q = -r$. It turns out, however, that the Cauchy-Schwarz inequality suffices in these cases. Moreover, the assumptions* (4.2.3) *implies that the special cases are only present if $p, q, r \in P_L$, in which case*

$$|\langle a_p^+ a_q^+ a_r \rangle| \leq Q(p,q)^{1/2}Q(r)^{1/2} \leq C \begin{cases} h_{2p}^{1/2}|s_p| & p = q \\ h_p h_{2p}^{1/2} & p = -r \\ h_q h_{2q}^{1/2} & q = -r \end{cases}.$$

It follows that the contribution to the energy per particle from the special cases is $\mathcal{O}(s_c^{1/2}\rho N^{-1/2}J_0)$.

Proposition 4.4.3. *We have*

$$\frac{\langle H_{A1}\rangle}{N} = -4K_0\hat{\varphi}_0\rho + \mathcal{O}\big(\Omega_{A_1}\big), \tag{4.4.4}$$

where

$$\Omega_{A1} := \rho K^2 + \rho J_0\big[\sqrt{\delta}\tilde{I}(Is_c + \delta\tilde{I}) + J_0 s_c(I + N^{-1}) + s_c N^{-1/2}\big]$$
$$+ \begin{cases} \rho K\big[\varepsilon_H + R_H^{-2} + R_L + L^{-1}\ln(L) + \tilde{W}\big] + \rho S|\ln(\varepsilon_H)|, & n = 3 \\ \rho K\big[\varepsilon_H^{n-2} + R_H^{-2} + \varepsilon_H R_L + L^{-1} + \tilde{W}\big] + \rho S, & n \geq 4 \end{cases}.$$

Proof. Notice that $\sqrt{N_0/N} = 1 + \mathcal{O}(K)$. Then, From Lemma 4.4.1 and Remark 4.4.2 above we arrive at the following estimate on the energy per particle of H_{A1}:

$$\frac{\langle H_{A1}\rangle}{N} = \big[1 + \mathcal{O}(K)\big]\frac{4\rho}{N^2}\sum_{\substack{p,q\in P_H\\ p+q\in P_L}} \hat{V}_q h_{p+q}\mathrm{Re}\left(\sqrt{c_p}\sqrt{c_q}\right) + \mathcal{O}(\tilde{\Omega}_{A1}) \tag{4.4.5}$$

where

$$\tilde{\Omega}_{A1} := \rho J_0\big[\sqrt{\delta}\tilde{I}(Is_c + \delta\tilde{I}) + J_0 s_c(I + N^{-1}) + s_c N^{-1/2}\big].$$

Suppose that $p, q \in P_H$ with $r := p + q \in P_L$. We claim that

$$\mathrm{Re}\left(\sqrt{c_p}\sqrt{c_q}\right) = -\rho\hat{w}_q + \mathcal{O}\big[|c_p + \rho\hat{w}_p| + |c_q + \rho\hat{w}_q| + \rho|r|(|q|^{-2} + |q|^{-3})\big]. \tag{4.4.6}$$

To see this, first notice that

$$\big|\mathrm{Re}\left(\sqrt{c_p}\sqrt{c_q}\right) + \rho\hat{w}_q\big| \leq \big|\sqrt{c_p}\sqrt{c_q} - c_q\big| + \big|c_q + \rho\hat{w}_q\big|.$$

Now, if c_p and c_q have different sign, then $|c_p| + |c_q| = |c_p - c_q|$ and hence

$$\big|\sqrt{c_p}\sqrt{c_q} - c_q\big| \leq \sqrt{|c_p|\,|c_q|} + |c_q| \leq 2|c_p - c_q|.$$

In case c_p and c_q have the same sign, we have

$$\big|\sqrt{c_p}\sqrt{c_q} - c_q\big| = \sqrt{|c_q|}\cdot\big|\sqrt{|c_p|} - \sqrt{|c_q|}\big| \leq \big|c_p - c_q\big|,$$

so in either case

$$\big|\sqrt{c_p}\sqrt{c_q} - c_q\big| \leq 2|c_p - c_q|. \tag{4.4.7}$$

Recall the estimate

$$\big|\hat{w}_{p+v} - \hat{w}_p\big| \leq C|v|\big(|p|^{-2} + |p|^{-3}\big), \tag{4.4.8}$$

for each $p, v \in \mathbb{R}^n$ with $|v|/|p| \leq c < 1$. Then (4.4.6) follows from the triangle inequality and (4.4.8). As a consequence the factor $\mathrm{Re}\left(\sqrt{c_p}\sqrt{c_q}\right)$ in (4.4.5) can be replaced by $-\rho\hat{w}_q$ by at cost of an error $\mathcal{O}[\rho K W_1 + \rho^2 S|\ln\varepsilon_H|]$ in three dimensions and $\mathcal{O}[\rho K W_1 + \rho^2 S]$ in higher dimensions. Furthermore, the summation over $p, q \in P_H$ with $p+q \in P_L$ can be replaced by the summation over $P_H \times P_L$ at the cost of an error $\mathcal{O}(\rho K R_L)$ in three dimensions and $\mathcal{O}(\rho K\varepsilon_H R_L)$ in higher dimensions. Finally, we note that since $\hat{V} * \hat{w} = (2\pi)^n\hat{\varphi}$, we have

$$\frac{1}{|\Lambda|}\sum_{q\in P_H}\hat{V}_q\hat{w}_q = \hat{\varphi}_0 + \mathcal{O}(\varepsilon_H^{n-2} + R_H^{-2} + \mathcal{E}_n(L)),$$

and the result follows. □

4.4.2 Interactions with Four Non-zero Momenta

In this section we estimate the energy of

$$H_{A2} = \frac{1}{2|\Lambda|} \sum_{(p,q,r,s)\in\mathcal{R}} \hat{V}_{p-r} a_p^+ a_q^+ a_r a_s, \tag{4.4.9}$$

where

$$\mathcal{R} := \big\{(p,q,r,s) \in (\Lambda^*\backslash\{0\})^4 : p+q = r+s,\ p \neq -q, r, s\big\}.$$

As for the interactions with three non-zero momenta, we begin by noting that, since $a_p^+ a_q^+ a_r a_s$ breaks symmetry in p, q, r, s, only terms with $p, q, r, s \in P_L \cup P_H$ give nonzero contribution to the expectation of (4.4.9) in our trial state. Moreover, since each $\alpha \in M$ represents a state with an even number of particles in P_H, we may assume that P_H contains exactly either zero, two or four of the momenta's p, q, r, s. This leads to a decomposition

$$H_{A2} = H_{A2}^0 + H_{A2}^2 + H_{A2}^4.$$

Throughout this section we let

$$T\alpha = T_{p,q,r,s}\alpha := \alpha + \delta_p + \delta_q - \delta_r - \delta_s.$$

Using the strategy from the proof of Lemma 4.4.1 in the case $p, q, r \in P_L$ (only here we have to partition M into 16 different regimes), we obtain

$$\langle a_p^+ a_q^+ a_r a_s\rangle = \mathcal{O}\big[|s_p s_q s_r s_s|\big(I^2 + IN^{-1} + N^{-2}\big)\big],$$

whenever $p, q, r, s \in P_L$ are $\pm$ different. The special cases are easily estimated by the Cauchy-Schwarz inequality. This leads to the following estimate on H_{A2}^0.

Lemma 4.4.4. *We have*

$$\frac{\langle H_{A2}^0\rangle}{N} = \mathcal{O}\big[\rho s_c J_0^3 (NI^2 + I + N^{-1})\big].$$

Lemma 4.4.5. *We have*

$$\frac{\langle H_{A2}^2\rangle}{N} = \mathcal{O}\bigg[\rho\delta^{1/2}\tilde{I}\big[K^2 + \delta I J_0 (J_0 + \delta K) N + \delta(K + J_0)\big]\bigg]. \tag{4.4.10}$$

Proof. Suppose first that $p, q \in P_L$ and $r, s \in P_H$. The only special case possible is $p = q$, in which case the Cauchy-Schwarz inequality yields

$$|\langle a_p^+ a_p^+ a_r a_s\rangle| \le Q(p,p)^{1/2} Q(r,s)^{1/2} \le C\delta |s_p| \sqrt{|c_r c_s|}.$$

Suppose now that $p \neq q$ (and hence p, q, r, s are $\pm$ different). Then

$$\langle a_p^+ a_q^+ a_r a_s\rangle = \sum_\alpha \overline{f(T\alpha)} f(\alpha) R_{r,s}^{p,q}(\alpha). \tag{4.4.11}$$

Decompose M into 4 regimes,

$$M_1 = M_p^s \cap M_q^s, \quad M_2 = M_p^s \cap M_q^a, \quad M_3 = M_p^a \cap M_q^s, \quad M_4 = M_p^a \cap M_q^a.$$

For $\alpha \in M_1$ we have the relation

$$f(T\alpha) = \frac{4}{N}\frac{c_p c_q}{\sqrt{c_r}\sqrt{c_s}} R^{p,q}(\alpha) f(\alpha),$$

and hence the contribution to (4.4.11) from this regime is

$$\begin{aligned}\Big|\sum_{\alpha\in M_1}\cdots\Big| &= \frac{4}{N}\frac{|c_p c_q|}{\sqrt{|c_r c_s|}}\sum_{\alpha\in M_1}(\alpha(p)+1)(\alpha(q)+1)R_{r,s}(\alpha)|f(\alpha)|^2 \\ &\le \frac{4}{N}\frac{|s_p s_q|}{\sqrt{|c_r c_s|}} Q(r,s) \le CN^{-1}\delta^2|s_p s_q|\sqrt{|c_r c_s|}.\end{aligned}$$

Next, for $\alpha \in M_2$,

$$f(T\alpha) = \frac{c_p}{\sqrt{c_r}\sqrt{c_s}}\sqrt{\frac{\alpha(p)+1}{\alpha(q)+1}} f(\alpha),$$

and hence

$$\begin{aligned}\Big|\sum_{\alpha\in M_2}\cdots\Big| &= \frac{|c_p|}{\sqrt{|c_r c_s|}}\sum_{\alpha\in M_2}|f(\alpha)|^2(\alpha(p)+1)R_{r,s}(\alpha) \\ &\le \frac{|s_p|}{\sqrt{|c_r c_s|}}\sum_{\alpha\in M_q^a}|f(\alpha)|^2\alpha(r)\alpha(s) \\ &\le CI\delta^2|s_p|h_q\sqrt{|c_r c_s|}.\end{aligned}$$

In the last inequality, the factor Ih_q comes from the fact that M_q^a is generated from M_q^s via soft-pair creations. The contribution from M_3 equals the contribution from M_2 with p and q interchanged. For the last case we use

$$\sum_{\alpha\in M_4}\cdots = \sum_{\beta\in M_1}\overline{f(\beta)}f(T^{-1}\beta)\sqrt{\beta(p)\beta(q)(\beta(r)+1)(\beta(s)+1)}$$

to obtain

$$\Big|\sum_{\alpha\in M_4}\cdots\Big| \le CN^{-1}h_p h_q\sqrt{|c_r|}\sqrt{|c_s|}.$$

In total we have

$$|\langle a_p^+ a_q^+ a_r a_s\rangle| \le C\sqrt{|c_r c_s|}\Big[N^{-1}h_p h_q + I\delta^2(h_q|s_p| + h_p|s_q|) + \delta^2 N^{-1}|s_p s_q|\Big].$$

The case $p, r \in P_L$ and $q, s \in P_H$ is similar: In the special case $p = -r$ we have

$$|\langle a_p^+ a_q^+ a_{-p} a_s\rangle| \le C\delta h_p\sqrt{|c_q c_s|},$$

and otherwise

$$|\langle a_p^+ a_q^+ a_r a_s\rangle| \le C\sqrt{|c_q c_s|}\Big[\delta N^{-1}\big(|s_p|h_r + h_p|s_r|\big) + \delta I|s_p s_r|\Big].$$

By carrying out the appropriate integrations, we arrive at the desired. □

Lemma 4.4.6. *Suppose that $\delta^2\rho^{-1}|\Lambda|R_L^{3n/2}R_H^{n/2} \le \rho^\varepsilon$, for some $\varepsilon > 0$. Then*

$$\frac{\langle H_{A2}^4\rangle}{N} = \frac{2\rho K_0}{(2\pi)^n}\int \hat{\varphi}_p\hat{w}_p\,dp + \mathcal{O}(\Omega_{A2}^4), \tag{4.4.12}$$

where

$$\begin{aligned}\Omega_{A2}^4 := {}& \rho\delta\tilde{I}^2\big[\delta^2 + K(Ih_c+\delta^2)\big] + R_H^{3n}\delta^4\rho^{-2}\big[1+\rho^{-1}h_c^2R_L^n\big]\\ &+ \rho K W_1\big[1+I_1+\delta^{1/2}\tilde{I}\big] + \rho K\big[\varepsilon_H^{n-2} + R_H^{-2} + \mathcal{E}_n(L)\big]\\ &+ \rho S\big[I_1+\delta^{1/2}\tilde{I}\big]\times\begin{cases}\big[R_H+\ln(R_H/\varepsilon_H)\big], & n=3\\ \big[R_H^{n-2}+R_H^{n-3}\big], & n\ge 4\end{cases}.\end{aligned}$$

Proof. Notice that, for $p,q,r,s\in P_H$,

$$f(T\alpha) = \frac{\sqrt{c_p}\sqrt{c_q}}{\sqrt{c_r}\sqrt{c_s}}f(\alpha),$$

whenever $T\alpha\in M$. There are essentially only two special cases to consider, namely $p=q$ and $p=-r$, and it is easy to see that

$$|\langle a_p^+a_q^+a_ra_s\rangle| \le C\delta^2|c_p|\begin{cases}\sqrt{|c_rc_s|} & \text{if } p=q\\ \sqrt{|c_qc_s|} & \text{if } p=-r\end{cases}.$$

It follows that the contribution to the energy per particle from the special cases is $\mathcal{O}(\delta^3\rho\tilde{I}^2)$. Now fix $(p,q,r,s)\in\mathcal{R}$ such that $p,q,r,s\in P_H$ are $\pm$ different. Then

$$\langle a_p^+a_q^+a_ra_s\rangle = \sum_\alpha \overline{f(T\alpha)}f(\alpha)R_{r,s}^{p,q}(\alpha) = A+B,$$

where

$$A := \sum_{\alpha\in M'}\overline{f(T\alpha)}f(\alpha)R_{r,s}^{p,q}(\alpha),\quad B := \sum_{\alpha\in M\setminus M'}\overline{f(T\alpha)}f(\alpha)R_{r,s}^{p,q}(\alpha)$$

and $M' := \mathcal{A}^{r+s,r}(M_{r+s}^s)$, if $r+s\in P_L$, and $M' := \emptyset$ otherwise. We will see that the main contribution comes from the term A. Suppose that $r+s\in P_L$. Since $T = \mathcal{A}^{p+q,p}\mathcal{A}_{r+s,r}$, we have

$$\begin{aligned}A &= \sum_{\beta\in M_{r+s}^s}\overline{f(\mathcal{A}^{p+q,p}\beta)}f(\mathcal{A}^{r+s,r}\beta)R^{r,s}(\beta)R^{p,q}(\beta)\\ &= \pm 4N^{-1}\sqrt{c_p}\sqrt{c_q}\sqrt{c_r}\sqrt{c_s}h_{p+q}\sum_{\beta\in M_{p+q}^s}|f(\beta)|^2R^{r,s}(\beta)R^{p,q}(\beta),\end{aligned}$$

where the negative sign applies in case c_p and c_q have different sign. From (4.3.9) it follows that

$$0 \le \sqrt{(a+1)(b+1)(c+1)(d+1)} - 1 \le \frac{1}{2}\big(ab+a+b+cd+c+d\big),$$

for nonnegative a, b, c, d. Using this fact and (4.3.8) we obtain

$$A = \pm 4N^{-1}\sqrt{c_p}\sqrt{c_q}\sqrt{c_r}\sqrt{c_s}h_{p+q} + \mathcal{O}\bigg(N^{-1}h_{p+q}|c_pc_qc_rc_s|^{1/2}\big[\delta(|c_r|+|c_s|+|c_p|+|c_q|)+Ih_{p+q}\big]\bigg). \tag{4.4.13}$$

With two integrations over P_H and one integration over P_L, the contribution to the energy per particle from the error in (4.4.13) is of order $\rho\delta\tilde{I}^2K(Ih_c+\delta^2)$. Using the triangle inequality, (4.4.7) and (4.4.8), we obtain

$$\begin{aligned}\pm\sqrt{c_p}\sqrt{c_q}\sqrt{c_r}\sqrt{c_s} = \rho^2\hat{w}_p\hat{w}_r + \mathcal{O}\Big\{&|c_r|\,|c_p+\rho\hat{w}_p| + \rho|\hat{w}_p|\,|c_r+\rho\hat{w}_r| \\ &+ \sqrt{|c_rc_s|}\big(|c_p+\rho\hat{w}_p| + \rho|p+q|(|p|^{-2}+|p|^{-3}) + |c_q+\rho\hat{w}_q|\big) \\ &+ |c_p|\big(|c_r+\rho\hat{w}_r| + \rho|r+s|(|r|^{-2}+|r|^{-3}) + |c_s+\rho\hat{w}_s|\big)\Big\}.\end{aligned} \tag{4.4.14}$$

The contribution to the energy per particle from the error in (4.4.14) is of order

$$\rho KW_1\big(1+I_1+\delta^{1/2}\tilde{I}\big) + \rho S\big(I_1+\delta^{1/2}\tilde{I}\big) \times \begin{cases} \big[R_H+\ln(R_H/\varepsilon_H)\big], & n=3 \\ \big[R_H^{n-2}+R_H^{n-3}\big], & n\geq 4 \end{cases}.$$

Furthermore, we have

$$\frac{2}{N^3}\sum_{\substack{p,q,r,s\in P_H\\ p+q=r+s}} \hat{V}_{p-r}\hat{w}_r\hat{w}_ph_{p+q} = \frac{2\rho K_0}{(2\pi)^3}\int\hat{\varphi}_p\hat{w}_p\,dp + \mathcal{O}\Big[\rho K\big(\varepsilon_H^{n-2}+R_H^{-2}+\mathcal{E}_n(L)\big)\Big].$$

In order to estimate the term B we employ the fact that

$$\sum_{\alpha(r)\geq m}|f(\alpha)|^2R_{r,s}^{p,q}(\alpha) = \mathcal{O}\big[\delta|c_s|(\delta|c_r|)^m\big], \quad m\geq 0, \tag{4.4.15}$$

and the analogues bounds for sums over $\alpha(s)\geq m$, $\alpha(p)\geq m$ and $\alpha(q)\geq m$. These estimates are easy, but tedious, to obtain using the strategy of Lemma 4.3.2 and $|c_p|\leq\delta$, for $p\in P_H$. As a consequence we may restrict attention to α's which are bounded uniformly in p,q,r,s, and hence it suffices to show that

$$\tilde{B} := \sum_{\alpha\in M\setminus M'}|f(T\alpha)f(\alpha)|$$

is negligible. Given $m\in\mathbb{N}_0$, a nonempty subset $\{v_1,\ldots,v_t\}\subset P_L$ of $\pm$ different elements and a $\gamma\in M$ with $\gamma(-v_i)=\gamma(v_i)\geq 1$, we let $M(m,\{v_1,\ldots,v_t\},\gamma)$ denote the set of all $\alpha\in M\setminus M'$ such that α and $T\alpha$ have the form

$$\alpha = \prod_{i=1}^t\mathcal{A}^{v_i,k_i}\prod_{j=1}^m\mathcal{A}^{q_j}\gamma, \quad T\alpha = \prod_{i=1}^t\mathcal{A}^{v_i,k_i'}\prod_{j=1}^m\mathcal{A}^{q_j'}\gamma. \tag{4.4.16}$$

Here $q_j, k_i, (v_i - k_i)$ are in P_H and similarly for the 'primes'. We also require that

$$k_i \neq k_i' \quad \text{and} \quad q_j \neq q_j'. \tag{4.4.17}$$

In case $m = 0$ the products over j in (4.4.16) should be interpreted as a factor one. Notice also that if $m = 0$, then $t \geq 2$, since otherwise $\alpha \in M'$. From the definition of f and the fact that $|c_k| \leq \delta$ whenever $k \in P_H$, we see that, for $\alpha \in M(m, \{v_1, \ldots, v_t\}, \gamma)$,

$$|f(T\alpha)f(\alpha)| \leq \delta^{2m}\big[4\delta^2 N^{-1}\big]^t |f(\gamma)|^2 \prod_{i=1}^{t} \gamma(v_i).$$

Since α and $T\alpha$ agree outside P_H and represent states with equal number of particles in P_H, it follows that

$$\{\alpha \in M \backslash M' : T\alpha \in M\} \subseteq \bigcup_{m,\{v_1,\ldots,v_t\},\gamma} M(m, \{v_1, \ldots, v_t\}, \gamma),$$

and hence we have an upper bound

$$\tilde{B} \leq \sum_{m,\{v_1,\ldots,v_t\},\gamma} \delta^{2m}\big[4\delta^2 N^{-1}\big]^t |f(\gamma)|^2 \prod_{i=1}^{t} \gamma(v_i) \cdot |M(m, \{v_1, \ldots, v_t\}, \gamma)|,$$

where $|\cdot|$ denotes the cardinality. We claim that

$$|M(m, \{v_1, \ldots, v_t\}, \gamma)| \leq |P_H|^{-1} t! \big[Ct|P_H|\big]^{t/2} \cdot \big[C|P_H|\big]^{m/2}, \tag{4.4.18}$$

if there exists an $i \in \{1, \ldots, t\}$ such that

$$v_i \in \operatorname{span}_{\{0,\pm 1\}} \{v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_t, p, q, r, s\}, \tag{4.4.19}$$

and $|M(m, \{v_1, \ldots, v_t\}, \gamma)| = 0$ otherwise. Here $\operatorname{span}_{\{0,\pm 1\}}$ denotes the set of all linear combinations with coefficients in $\{0, 1, -1\}$. To verify (4.4.18) we suppose that $\alpha \in M(m, \{v_1, \ldots, v_t\}, \gamma)$ so that α and $T\alpha$ has the form (4.4.16). Since in particular $\alpha \notin M'$ we must have

$$\{k_i, v_i - k_i\} \neq \{r, s\} \quad \text{and} \quad \{k_i', v_i - k_i'\} \neq \{p, q\}. \tag{4.4.20}$$

Since $T\alpha(k) = \alpha(k)$, for each $k \notin \{p, q, r, s\}$, the P_H-momenta in the representation for α respectively $T\alpha$ in (4.4.16) are almost the same. We denote the common momenta by $p_1, \ldots, p_{2(m+t)-2}$. Counting with multiplicity, the P_H-momenta appearing in (4.4.16) for α respectively $T\alpha$ can then be listed as

$$\begin{array}{llllll} \alpha: & r, & s, & p_1, & \ldots, & p_{2(m+t)-2} \\ T\alpha: & p, & q, & p_1, & \ldots, & p_{2(m+t)-2} \end{array}$$

Thus each common momenta appear in *one* α-pair and *one* $T\alpha$-pair. By (4.4.20), the momenta p, q, r, s form pair with one common momenta each. A 'graph' is associated

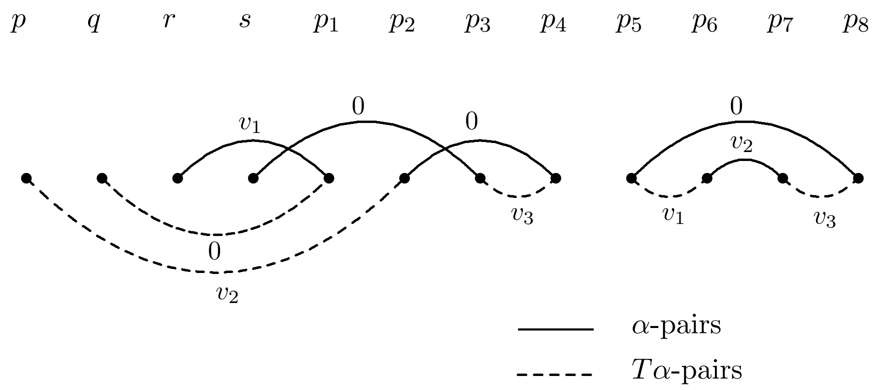

Figure 4.1: A visualization of typical α- and $T\alpha$-pairs in the case $m = 3$ and $t = 2$.

to α as follows (see Figure 4.1): We represent each P_H-momentum pair from (4.4.16) by two dots connected by an arc, labeled by the sum of the momenta's in the pair (so in particular we can distinguish strict pairs from soft-pairs). The graph consists of two chains (parts involving p, q, r, s) and possibly a number of loops (parts involving only common momenta). Since the ends of the chains are fixed, and since chains must involve soft-pairs (since p, q, r, s are $\pm$ different), it follows that (4.4.19) holds, for some i. The *length* of a chain/loop is the number of points in it. Suppose that the graph has a total of $l \geq 2$ chains and loops with respective lengths $m_1, \ldots m_l$. Then we must have

$$m_1 + \ldots + m_l = 2(m + t) + 2. \tag{4.4.21}$$

By (4.4.17), each loop has length a least 4. Since the two chains contain at least one of the p_i's each, it follows that

$$l - 2 \leq \frac{2(m+t) - 2 - 2}{4} = \frac{m+t}{2} - 1. \tag{4.4.22}$$

We call a chain or a loop *trivial* if all associated $T\alpha$ -pairs are strict. Since each trivial chain involves at least one strict pair and each trivial loop involves at least two strict pairs, it follows that the total number of trivial chains and loops are at most $m/2 + 1$. Hence the number of non-trivial chains and loops is at least $l - (m/2 + 1)$. Thus we can bound the number of $\alpha \in M(m, \{v_1, \ldots, v_t\}, \gamma)$ having the particular graph above as follows:

- Choose one p_i in each loop. The total number of choices is less than $|P_H|^{l-2}$
- Choose the positions of the m zero's in the $m + t$ α-edges. The total number of choices is less than 2^{m+t}
- Choose the positions of $v_1, \ldots, v_t$ in the remaining t α-edges. The total number of choices is $t!$

- Choose the positions of the m zero's in the $m+t$ $T\alpha$-edges. The total number of choices is less than 2^{m+t}
- Choose the positions of the v_i's in $T\alpha$-edges. The total number of choices is less than $t^{t-(l-m/2-1)}$

Taking the product of the above yields

$$4^{m+t}t!|P_H|^{-2}t^{t+m/2+1}\big(|P_H|/t\big)^l \leq |P_H|^{-1}t!\big[16t|P_H|\big]^{t/2}\big[16|P_H|\big]^{m/2}, \tag{4.4.23}$$

where the inequality follows from (4.4.22), assuming that $|P_H|/t \geq 1$. Since the right-hand side in (4.4.23) is independent of $m_1,\dots,m_l$ and l, we only need to show that the number of different graphs is bounded by C^{m+t}. But this follows by considering (for fixed l) the number of nonnegative integer solutions to (4.4.23), summing from $l = 2,\dots,(m+t)/2+1$ and then using the binomial theorem.

Employing the bound (4.4.18) we now can finish the proof as follows: First perform the summation over γ,

$$\sum_{\gamma\in\cap_i M^s_{v_i}} |f(\gamma)|^2 \prod_{i=1}^t \gamma(v_i) \leq h_c^t \sum_{\gamma\in\cap_i M^s_{v_i}} |f(\gamma)|^2 \leq h_c^t. \tag{4.4.24}$$

Next we note that, for fixed t, the number of subsets $\{v_1,\dots,v_t\} \subset P_L$ with the property that (4.4.19) holds, for some i, is bounded by

$$t3^{t+3}\frac{|P_L|^{t-1}}{(t-1)!}.$$

Thus we have

$$\begin{aligned}\tilde{B} &\leq \frac{C}{|P_L|\cdot|P_H|}\sum_{t\geq 1}\sum_{\substack{m\geq 0\\ m+t\geq 2}} \big[C\delta^2|P_H|^{1/2}\big]^m\big[C\delta^2 h_c N^{-1}|P_L|(t|P_H|)^{1/2}\big]^t \\ &\leq C\delta^4 N^{-1} + \frac{C}{|P_L|\cdot|P_H|}\sum_{t\geq 2}\big[C\delta^2 h_c N^{-1}|P_L|(t|P_H|)^{1/2}\big]^t.\end{aligned}$$

Let $t_0 \geq 2$ and notice that

$$\sum_{2\leq t\leq t_0}\big[C\delta^2 h_c N^{-1}|P_L|(t|P_H|)^{1/2}\big]^t \leq Ct_0\delta^4 h_c^2|P_L|^2|P_H|N^{-2},$$

provided $\delta^2 h_c N^{-1}|P_L|(t_0|P_H|)^{1/2}$ is sufficiently small (which is true if μ below is small). For the remaining part of the sum, we use $t \leq |P_L|$ to obtain

$$\sum_{t>t_0}\big[C\delta^2 h_c N^{-1}|P_L|(t|P_H|)^{1/2}\big]^t \leq C\mu^{t_0},$$

provided

$$\mu := C\delta^2 h_c N^{-1}|P_L|^{3/2}|P_H|^{1/2}$$

is sufficiently small. In total we get

$$\frac{\tilde{B}|P_H|^3}{N|\Lambda|} \leq \left(\frac{|P_H|}{|\Lambda|}\right)^3 \left[\delta^4\rho^{-2} + t_0\delta^4\rho^{-3}h_c^2\frac{|P_L|}{|\Lambda|} + \frac{|\Lambda|}{|P_H||P_L|}\rho^{-1}\mu^{t_0}\right]$$

From the bounds $|P_L| \sim |\Lambda|R_L^n$ and $|P_H| \sim |\Lambda|R_H^n$ we see that

$$\left|\frac{1}{N|\Lambda|}\sum_{\substack{p,q,r,s\in P_H\\ p+q=r+s}} \tilde{B}\right| \leq CR_H^{3n}\delta^4\rho^{-2}\big(1+\rho^{-1}h_c^2R_L^n\big),$$

provided $\mu \leq \rho^\varepsilon$ and t_0 sufficiently large. Also notice that

$$\mu \leq C\delta^2\rho^{-1}|\Lambda|R_L^{3n/2}R_H^{n/2}.$$

By adding up the error terms we are finally done. □

4.5 Minimization and Estimates

Considering (4.3.13) we start by noting that

$$\frac{2\rho}{N}\sum_{p\neq 0}\hat{\varphi}_p h_p = 2\rho K_0\hat{\varphi}_0 + \mathcal{O}\big[\rho(K-K_0)+\rho S\big]. \tag{4.5.1}$$

For the excess kinetic energy we have

$$\begin{aligned}\frac{1}{N}\sum_{p\in P_H} p^2\tilde{h}_p &= \big[1+\mathcal{O}(\delta^2)\big]\frac{4}{N^2}\sum_{p\in P_H}p^2|s_p|\sum_{\substack{v\in P_L\\ v-p\in P_H}}|c_{v-p}|h_v \\ &= \big[1+\mathcal{O}(\delta^2)\big]\left(\frac{2K_0\rho}{(2\pi)^n}\int \hat{g}_p\hat{w}_p\,dp + \mathcal{O}(\Omega_{\text{Kin}})\right),\end{aligned} \tag{4.5.2}$$

where

$$\begin{aligned}\Omega_{\text{Kin}} &:= \frac{1}{N^2}\sum_{p\in P_H}\sum_{\substack{v\in P_L\\ v-p\in P_H}} p^2|s_p|\big|c_{v-p}-c_p\big|h_v + \frac{K}{N}\sum_{\varepsilon_H\leq|p|\leq\varepsilon_H+R_L} p^2h_p \\ &+ \frac{K}{N}\sum_{R_H-R_L\leq|p|\leq R_H} p^2h_p + \frac{K\rho}{|\Lambda|}\sum_{p\notin P_H}\hat{g}_p\hat{w}_p \\ &+ \frac{K}{N}\sum_{p\in P_H}p^2\big[h_p-(\rho\hat{w}_p)^2\big] + K\rho\mathcal{E}_n(L).\end{aligned}$$

Upon adding the (presumable) main terms from (4.5.1), (4.5.2), (4.4.12) and (4.4.4), and by using $(2\pi)^n\hat{\varphi} = \hat{V} * \hat{w}$, we see that they exactly cancel:

$$2\rho K_0\hat{\varphi}_0 + \frac{2K_0\rho}{(2\pi)^n}\int\hat{g}_p\hat{w}_p\,dp + \frac{2\rho K_0}{(2\pi)^3}\int\hat{\varphi}_p\hat{w}_p\,dp - 4K_0\hat{\varphi}_0\rho = 0.$$

We choose the function e_p pointwise to minimize the expression

$$m_p := \frac{e_p^2 + 2\rho\hat{w}_p e_p}{1 - 2e_p}.$$

from (4.3.14). This yields

$$-e_p^2 + e_p + \rho\hat{w}_p = 0, \quad e_p = \frac{1}{2}\Big(1 - \sqrt{1 + 4\rho\hat{w}_p}\Big) \tag{4.5.3}$$

and

$$m_p = \frac{1}{2}\big(\sqrt{1 + 4\rho\hat{w}_p} - 1 - 2\rho\hat{w}_p\big),$$

provided $1 + 4\rho\hat{w}_p \geq 0$. Note however that, since $\hat{g}$ is continuous, $\hat{g}_0 > 0$ and $\hat{g}_p \to 0$ as $|p| \to \infty$, it follows that $\hat{w}_p$ is bounded from below, and hence

$$\liminf_{\rho\to 0} \big[\inf_{p\neq 0}(1 + 4\rho\hat{w}_p)\big] \geq 1.$$

Notice that (4.5.3) yields

$$c_p = \frac{1 - \sqrt{1 + 4\rho\hat{w}_p}}{1 + \sqrt{1 + 4\rho\hat{w}_p}}, \quad s_p = \frac{-\rho\hat{w}_p}{\sqrt{1 + 4\rho\hat{w}_p}}, \quad h_p = \frac{1}{2}\bigg(\frac{1 + 2\rho\hat{w}_p}{\sqrt{1 + 4\rho\hat{w}_p}} - 1\bigg). \tag{4.5.4}$$

Also notice that

$$c_p = -\rho\hat{w}_p + \mathcal{O}((\rho\hat{w}_p)^2) \quad \text{as } \rho p^{-2} \to 0.$$

Finally, with the choice in (4.5.3) we have

$$E^{\mathrm{Bog}} = \frac{\hat{g}_0}{2}\rho + \frac{1}{2\rho|\Lambda|}\sum_{p\neq 0} p^2 \Phi(\rho\hat{w}_p), \tag{4.5.5}$$

where

$$\Phi(t) := \sqrt{1 + 4t} + 2t^2 - 2t - 1. \tag{4.5.6}$$

Notice that $\rho\hat{w}_p \leq \hat{g}_0\rho\varepsilon_L^{-2}/2$, for any $p \in P_L$. Suppose that $R_L \ll 1$ such that also $\rho\hat{w}_p > 0$ whenever $p \in P_L$. Then

$$s_c = \sup_{p\in P_L} |s_p| = \mathcal{O}(\rho^{1/2}\varepsilon_L^{-1})$$

In Table 4.2 we have listed elementary estimates on the quantities from Table 4.1, given the particular choice in (4.5.3) (see also [4] and Section 3.3.3).

4.5.1 Dimension $n = 3$

A straightforward calculation, using the fact that Φ is increasing and $\hat{g}_p \leq \hat{g}_0$, yields

$$E^{\mathrm{Bog}} \leq 4\pi a\rho\bigg(1 + \frac{128}{15\sqrt{\pi}}(a^3\rho)^{1/2}\bigg) + \mathcal{O}\big[\rho^{3/2}(\ln L)/L\big],$$

	I	J	K	S	T	U	W	J_0
$n=3$	$\rho\varepsilon_H^{-1}$	1	$\rho^{1/2}$	$\rho\ln\rho$	ρ	1	$\rho^{1/2}$	R_L
$n=4$	$\rho\varepsilon_H^{-1}$	1	$\rho\ln\rho$	ρ	ρ	1	$\rho\ln\rho$	R_L^2
	$\tilde{I}$	$\tilde{J}$	$\tilde{K}$	W_1	I_1	s_c	h_c	δ
$n=3$	$\rho^{-1/2}$	$\rho^{1/2}$	$\rho^{1/2}$	$\rho^{1/2}$	1	$\rho^{1/2}\varepsilon_L^{-1}$	$\rho^{1/2}\varepsilon_L^{-1}$	$\rho\varepsilon_H^{-2}$
$n=4$	$\rho^{-1/2}$	$\rho\ln\rho$	$\rho\ln\rho$	$\rho\ln\rho$	1	$\rho^{1/2}\varepsilon_L^{-1}$	$\rho^{1/2}\varepsilon_L^{-1}$	$\rho\varepsilon_H^{-2}$

Table 4.2: Estimates on the quantities from Table 4.1. The information here is that $I = \mathcal{O}(\rho\varepsilon_H^{-1})$, for $n=3$, and so on.

where the error $\rho^{3/2}(\ln L)/L$ comes from replacing the sum with an integral. We now choose parameters. From (4.5.1) we need $K \approx K_0$, and since the main contribution to the sum defining K comes from $|p| \sim \rho^{1/2}$, we choose $\varepsilon_L, R_L \sim \rho^{1/2}$. From Ω_{A1} in Proposition 4.4.3 and Ω_{A2} in Lemma 4.4.6, it is clear that we need $\varepsilon_H \ll 1$ and $R_H^{-1} \ll 1$. However, from the estimates on I and δ in Table 4.2 it is also clear that ε_H cannot be too small, which in turns implies that R_H cannot be too large. In particular, if we take $R_H = \varepsilon_H^{-1}$, then the second term in Ω_{A2} together with $\delta = \mathcal{O}(\rho\varepsilon_H^{-2})$ shows that $\varepsilon_H \geq \rho^{1/34}$. For simplicity we choose

$$\varepsilon_L = \rho^{1/2+\eta}, \quad R_L = \rho^{1/2-\eta}, \quad \varepsilon_H = \rho^{\eta} \quad \text{and} \quad R_H = \rho^{-\eta}$$

for some $0 < \eta \leq 1/34$. Moreover we take $L = \rho^{-(1+\eta)}$. With these choices we obtain

$$\Omega_P = \mathcal{O}(\rho^{2-3\eta}) \quad \text{and} \quad \Omega_{A1} = \mathcal{O}(\rho^{3/2+\eta}).$$

Furthermore, the contributions from Lemma 4.4.4 and Lemma 4.4.5 are $\mathcal{O}(\rho^{5/2-9\eta})$ respectively $\mathcal{O}(\rho^{2-9\eta})$. The condition in Lemma 4.4.6 is satisfied if $\eta < 1/52$ and the contribution is then $\Omega_{A2} = \mathcal{O}(\rho^{3/2+\eta})$. Finally, one can check that the errors from (4.5.1) and (4.5.2) are also of order $\rho^{3/2+\eta}$. This concludes the proof of Theorem 4.1.3.

4.5.2 Dimension $n = 4$

In 4 dimensions we have (see Section 3.3.3)

$$E^{\text{Bog}} \leq 4\pi^2 a^2 \rho \Big(1 + 2\pi^2 a^4 \rho |\ln(a^4\rho)|\Big) + \mathcal{O}\big[\rho^2(1 + |\ln\rho| L^{-1})\big].$$

Proceeding similarly to the 3-dimensional case, we seek parameters such that $K \approx K_0$. However, in 4 dimensions, the dominant part of $\sum_{p\neq 0} h_p$ comes from the regime $\rho^{1/2} \leq |p| \leq 1$, and hence we are forced to take $R_L \sim 1$. Furthermore, we have the estimate

$$\Omega_P = \mathcal{O}(\rho^2\varepsilon_H^{-3} + \rho L^{-1}),$$

similar to the 3-dimensional case, so we must also have $\varepsilon_H \sim 1$ and $L \sim \rho^{-1}$. On the other hand, since $J_0 = R_L^2$, we see that the estimates in Section 4.4.6 all require $R_L \sim \rho^{\alpha}$, for some $1/4 \leq \alpha \leq 1/2$. A further complication arises when we attempt to divide Λ into smaller boxes (since we cannot take the thermodynamic limit). With $L = \rho^{-\gamma}$, we could repeat the steps from Section 4.1 to show that

$$e_0(\rho) \leq 4\pi^2 a^2 \rho \Big(1 + 2\pi^2 a^4 \rho |\ln(a^4\rho)| \Big) + \Omega + C\rho^{1/2+\gamma},$$

where Ω denotes the sum of all 'error terms'. Thus, in 4 dimensions we need $\gamma \approx 3/2$, in contrast to $\gamma \approx 1$ in 3 dimensions. This makes an appropriate choice of parameters even harder, if not impossible.

4.A Proof of Lemma 4.1.1

Define the function $q : \mathbb{R} \to [0,1]$ by

$$q(t) = \begin{cases} \cos\left[\frac{\pi(t-l)}{4l}\right] & |t| \leq l \\ 1 & l < t < L-l \\ \cos\left[\frac{\pi(t-(L-l))}{4l}\right] & |t-L| \leq l \\ 0 & \text{otherwise} \end{cases}.$$

Suppose that $\psi \in L^2_{\text{loc}}(\mathbb{R})$ is L-periodic. By definition of q,

$$\begin{aligned} \int_{-l}^{L+l} |q(t)\psi(t)|^2 \, dt &= \int_{-l}^{l} \cos^2\left(\frac{\pi(t-l)}{4l}\right) |\psi(t)|^2 \, dt + \int_{l}^{L-l} |\psi(t)|^2 \, dt \\ &+ \int_{L-l}^{L+l} \cos^2\left(\frac{\pi[t-(L-l)]}{4l}\right) |\psi(t)|^2 \, dt. \end{aligned}$$

In the latter integral we now employ a change of variables $s = t - L$ (which leaves ψ invariant) and the identity $\cos(\theta + \pi/2) = -\sin\theta$, to obtain

$$\int_{L-l}^{L+l} \cos^2\left(\frac{\pi[t-(L-l)]}{4l}\right) |\psi(t)|^2 \, dt = \int_{-l}^{l} \sin^2\left(\frac{\pi(t-l)}{4l}\right) |\psi(t)|^2 \, dt.$$

Hence, in total

$$\int_{-l}^{L+l} |q(t)\psi(t)|^2 \, dt = \int_{0}^{L} |\psi(t)|^2 \, dt, \tag{4.A.1}$$

showing that $\psi \mapsto q\psi$ is an isometry from $L^2_{\rm per}([0,L])$ to $L^2_{\rm Dir}([-l, L+l])$. Next we notice that

$$\int_{-l}^{L+l} |(q\psi)'(t)|^2\,dt = \int_{-l}^{L+l} |q(t)\psi'(t)|^2\,dt + 2\int_{-l}^{L+l} q(t)q'(t)\mathrm{Re}\,(\bar{\psi}(t)\psi(t))\,dt$$
$$+ \int_{-l}^{L+l} |q'(t)\psi(t)|^2\,dt$$
$$= \int_{0}^{L} |\psi'(t)|^2\,dt + 2\int_{-l}^{L+l} q(t)q'(t)\frac{d}{dt}|\psi(t)|^2\,dt$$
$$+ \int_{-l}^{L+l} |q'(t)\psi(t)|^2\,dt,$$

where we have used (4.A.1) and the fact that ψ' is periodic in the last equality. Notice that $|q'(t)| \leq Cl^{-1}\chi(t)$ and $|q''(t)| \leq Cl^{-2}\chi(t)$, where χ is the characteristic function of the set $[-l,l] \cup [L-l, L+l]$. Moreover, an integration by parts and the fact that $q(-l) = 0 = q(L+l)$ yields

$$\int_{-l}^{L+l} q(t)q'(t)\frac{d}{dt}|\psi(t)|^2\,dt = -\int_{-l}^{L+l} \left[q'(t)^2 + q(t)q''(t)\right]|\psi(t)|^2\,dt.$$

It follows that

$$\int_{-l}^{L+l} |(q\psi)'(t)|^2\,dt \leq \int_{0}^{L} |\psi'(t)|^2\,dt + Cl^{-2}\int |\psi(t)|^2\chi(t)\,dt.$$

Fix an arbitrary $u \in \mathbb{R}^n$ to be averaged out. We can generalize the above arguments to construct an isometry F^u from $L^2_{\rm per}([0,L]^{nN})$ into $L^2_{\rm Dir}([-l-u, L+l-u]^{nN})$ as follows. Let

$$h(x) = q(x^{(1)})\cdots q(x^{(n)}), \quad x = (x^{(1)},\dots,x^{(n)}) \in \mathbb{R}^n.$$

Then define

$$F^u(\Psi)(x_1,\dots,x_N) = \Psi(x_1,\dots,x_N)\prod_{i=1}^{N} h(x_i+u).$$

Then F^u is an isometry and furthermore

$$\|\nabla F^u(\Psi)\|^2_{L^2([-l-u,L+l-u]^{nN})} \leq \|\Psi\|^2_{L^2([0,L]^{nN})} + Cl^{-2}\sum_{i=1}^{N}\int \chi(x_i+u)|\Psi|^2,$$

where χ is now the characteristic function of the set $\{x \in \mathbb{R}^n : \mathrm{dist}(x, \partial[0,L]^n) \leq l)\}$. For the interaction energy we notice that $V(x) \leq V_L(x)$, since V is nonnegative. Then, using the isometry property of F^u, we have

$$\int |F^u(\Psi)|^2 V(x_j - x_k) \leq \int \left|F^u(\Psi\sqrt{V_L(x_j-x_k)})\right|^2 = \int |\Psi|^2 V_L(x_j - x_k).$$

In total we have shown the estimate

$$\langle H^{\rm Dir}_{N,L+2l}\rangle_{F^u(\Psi)} \leq \langle H^{\rm per}_{N,L}\rangle_\Psi + Cl^{-2}\sum_{i=1}^{N}\langle\chi(x_i+u)\rangle_\Psi,$$

for each $u \in \mathbb{R}^n$. By averaging over $u \in [0, L]^n$ we obtain

$$\int_{[0,L]^n} \langle H^{\text{Dir}}_{N,L+2l} \rangle_{F^u(\Psi)} \, du \le L^n \langle H^{\text{per}}_{N,L} \rangle_\Psi + CNL^{n-1} l^{-1} \|\Psi\|.$$

Thus, for each periodic Ψ there exists a $u \in [0, L]^n$, such that

$$\langle H^{\text{Dir}}_{N,L+2l} \rangle_{F^u(\Psi)} \le \langle H^{\text{per}}_{N,L} \rangle_\Psi + C \frac{N}{lL} \|\Psi\|. \tag{4.A.2}$$

Finally, the grand canonical version is obtained by applying (4.A.2) componentwise.

4.B Proof of Lemma 4.1.2

Fix an arbitrary $k \in \mathbb{N}$ and set $\tilde{L} = k(L + R)$. We place $M := k^n$ copies of Λ_L inside the larger box $\Lambda_{\tilde{L}}$, such that neighboring boxes are separated by a distance R. Denote the center of the j'th box by c_j. We may assume that $c_1 = 0$. Pick an arbitrary $\Psi \in H^1_0(\Lambda^N_L)$ and extend Ψ trivially to all of $\mathbb{R}^{nN}$. Define

$$\varphi_j(x_1, \ldots, x_N) := \Psi(x_1 - c_j, \ldots, x_N - c_j)$$

and

$$\Phi := \varphi_1(x_1, \ldots, x_N) \cdot \varphi_2(x_{N+1}, \ldots, x_{2N}) \cdots \varphi_M(x_{(M-1)N+1}, \ldots, x_{MN}).$$

Then Φ is an MN-particle Dirichlet function on the larger box, and by Tonelli's theorem and a simple change of variables, it follows that $\|\Phi\| = \|\Psi\|^M$. Moreover, we claim that

$$\langle \Phi, H_{MN,\tilde{L}} \Phi \rangle = M \|\Psi\|^{2(M-1)} \langle \Psi, H_{N,L} \Psi \rangle. \tag{4.B.1}$$

To see this, first split the kinetic energy into the M different sectors:

$$\|\nabla \Phi\|^2 = \sum_{i=1}^{N} \|\nabla_i \Phi\|^2 + \sum_{i=N+1}^{2N} \|\nabla_i \Phi\|^2 + \ldots + \sum_{i=(M-1)N+1}^{MN} \|\nabla_i \Phi\|^2.$$

Again, by Tonelli's theorem,

$$\begin{aligned} \sum_{i=1}^{N} \|\nabla_i \Phi\|^2 &= \int_{\Lambda^{(M-1)N}_{\tilde{L}}} |\Phi|^2 |\varphi_1|^{-2} \Big(\int_{\Lambda^N_L} \sum_{i=1}^{N} |\nabla_i \Psi|^2 \Big) \\ &= \|\Psi\|^{2(M-1)} \sum_{i=1}^{N} \|\nabla_i \Psi\|^2, \end{aligned}$$

and by a change of variables, we get identical contributions from the remaining $M - 1$ terms. For the interaction energy, we notice that, due to the spacing, particles in different boxes do not interact. By a similar argument as above we then see that

$$\int_{\Lambda^{MN}_{\tilde{L}}} \sum_{1 \le i < j \le MN} V(x_i - x_j) |\Phi|^2 = M \|\Psi\|^{2(M-1)} \int_{\Lambda^N_L} \sum_{1 \le i < j \le N} V(x_i - x_j) |\Psi|^2.$$

Now, for a grand-canonical Dirichlet wave function $\Psi^{\mathrm{GC}} = \oplus_{N=0}^{\infty} \Psi_N$ we apply the above construction componentwise to define Dirichlet functions Φ_{MN} on the larger box. Then

$$\Phi^{\mathrm{GC}} := \bigoplus_{N=0}^{\infty} \|\Psi_N\|^{1-M} \Phi_{MN}$$

readily satisfies $\|\Phi^{\mathrm{GC}}\| = \|\Psi^{\mathrm{GC}}\|$,

$$\langle \mathcal{N} \rangle_{\Phi^{\mathrm{GC}}} = M \langle \mathcal{N} \rangle_{\Psi^{\mathrm{GC}}} \quad \text{and} \quad \langle H_{\tilde{L}} \rangle_{\Phi^{\mathrm{GC}}} = M \langle H_L \rangle_{\Psi^{\mathrm{GC}}}.$$

Thus we have

$$\frac{\langle H_L \rangle_{\Psi^{\mathrm{GC}}}}{N} = \frac{\langle H_{\tilde{L}} \rangle_{\Phi^{\mathrm{GC}}}}{MN} \geq \frac{E_0^{\mathrm{GC}}(MN, \tilde{L})}{MN},$$

for each normalized Dirichlet state Ψ^{GC}, and hence

$$\frac{E_0^{\mathrm{GC}}(N, L)}{N} \geq \frac{E_0^{\mathrm{GC}}(MN, \tilde{L})}{MN}. \tag{4.B.2}$$

Now, the left-hand-side in (4.B.2) is independent of k, so the result follows from Lemma 3.3.2 in the the limit $k \to \infty$.

Bibliography

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

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

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

[4] L. Erdős, B. Schlein, and H-T. Yau. The ground state energy of a low density bose gas: a second order upper bound. *Phys. Rev. A*, 78, 2008.

[5] M. Girardeau and R. Arnowitt. Theory of many-boson systems: Pair theory. *Phys. Rev. 105*, 113:755–760, 1959.

[6] A. Giuliani and R. Seiringer. The ground state energy of the weakly interacting bose gas at high density. *J. Stat. Phys.*, 135:915–934, 2009.

[7] L. Grafakos. *Classical and Modern Fourier Analysis*. Prentice Hall, 1. edition, 2004.

[8] J. O. Lee and J. Yin. A lower bound on the ground state energy of a dilute bose gas. *J. Math. Phys.*, 51, 2010.

[9] T.D. Lee, K. Huang, and C.N. Yang. Eigenvalues and eigenfunctions of a bose system of hard spheres and its low-temperature properties. *Phys. Rev.*, 106:1135–1145, 1957.

[10] T.D. Lee and C.N. Yang. Many-body problem in quantum mechanics and quantum statistical mechanics. *Phys Rev.*, 105:119–120, 1957.

[11] E. Lieb, R. Seiringer, J.P. Solovej, and J. Yngvason. *The Mathematics of the Bose Gas and its Condensation*. Birkhäuser, 1. edition, 2005.

[12] E. H. Lieb and W. Liniger. Simplified approach to the ground-state energy of an imperfect bose gas. application to the one-dimensional model. *Phys. Rev.*, 134 2A, 1963.

[13] E. H. Lieb, R. Seiringer, and J. Yngvason. Bosons in a trap: A rigorous derivation of the gross-pitaevskii energy functional. *Phys. Rev. A*, 61 043602, 2000.

[14] E. H. Lieb and J. Yngvason. Ground state energy of the low density bose gas. *Phys. Rev. Lett.*, 80:2504–2507, 1998.

[15] E. H. Lieb and J. Yngvason. The ground state energy of a dilute two-dimensional bose gas. *J. Stat. Phys.*, 103:509–526, 2001.

[16] E.H. Lieb. The bose fluid. *Univ. of Colorado Press*, pages 175–224, 1964.

[17] C. Mora and Y. Castin. Ground state energy of the two-dimensional weakly interacting bose gas: First correction beyond bogoliubov theory. *Phys. Rev. Lett.*, 102, 2009.

[18] M.Reed and B. Simon. *Methods of Modern Mathematical Physics Vol. 4*. Academic Press, 1. edition, 1978.

[19] D. Ruelle. *Statistical Mechanics: Rigorous Results*. Imperial College Press and World Scientific, 3. edition, 1969.

[20] M. Schick. Two-dimensional system of hard core bosons. *Phys. Rev. A*, pages 1067–1073, 1971.

[21] B. Simon. *Convexity: An Analytical Viewpoint*. Cambridge University Press, 1. edition, 2011.

[22] J.P. Solovej. Upper bounds to the ground state energies of the one- and two-component charges bose gases. *Comm. Math. Phys.*, 266, 2006.

[23] J.P. Solovej. *Many Body Quantum Mechanics*. Lecture Notes, 2007.

[24] C. N. Yang. Pseudopotential method and dilute hard "sphere" bose gas in dimension 2,4 and 5. *Europhys. Lett.*, 84 40001, 2008.

[25] H-T. Yau and J. Yin. The second order upper bound for the ground state energy of a bose gas. *J. Stat. Phys.*, 2009.

[26] J. Yin. Quantum many-body systems with short-range interactions (ph.d. dissertation). *Princeton University.*, 2008.