Birger Brietzke

On the Second Order Correction to the Ground State Energy of the Dilute Bose Gas

PhD Thesis

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University of Copenhagen.

Birger Brietzke
Department of Mathematical Sciences
University of Copenhagen
Universitetsparken 5
DK-2100 København Ø
Denmark

Birger@math.ku.dk

Advisor:	Jan Philip Solovej University of Copenhagen, Denmark
Assessment committee:	Bergfinnur Duurhus (Chairman) University of Copenhagen, Denmark
	Robert Seiringer IST Austria, Austria
	Horia D. Cornean Aalborg University, Denmark

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Summary

In this thesis we consider a gas of interacting, identical, spin-less bosons in a thermodynamic box. We are interested in the ground state energy, which for low densities (diluteness) is described by the Lee–Huang–Yang (LHY) formula – a series expansion in the density that has been derived from Bogolubov's work in the late 1950's.
In the introduction we discuss how to derive the LHY formula using Bogolubov's approximation step, which presupposes Bose-Einstein condensation. The second part contains a detailed proof, which establishes the LHY formula as a lower bound in a *weak coupling* and *low density* regime. While our proof is guided by Bogolubov's predictions, it is based on a two-step localization procedure, which allows us to prove adequate 'local condensation'.

Resumé

I denne afhandling betragtes en gas af vekselvirkende, identiske bosoner uden spin i en termodynamisk boks. Vi er interesseret i grundtilstandsenergien, som for lave densiteter beskrives ved hjælp af Lee–Huang–Yang (LHY) formlen – en rækkeudvikling i densiteten, som blev udledt fra Bogolubovs arbejde i slutningen af 1950'erne.
I introduktionen diskuteres en udledning af LHY-formlen baseret på Bogolubovs approksimation, som forudsætter Bose-Einstein-kondensation. I anden del af afhandlingen præsenteres et detaljeret bevis, som etablerer LHY-formlen som nedre grænse i et regime med *svag kopling* og *lav densitet*. Vores bevis tager afsæt i Bogolubovs forudsigelser, men er baseret på en to-trins lokaliseringsprocedure, som tillader os at vise en passende form for 'lokal kondensation'.

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Part I

Introduction

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the one for interacting bosons without entropy
in the density limit – the dilute
we calculate a constant
hopefully important
using operators – which do not commute

– B. Brietzke

1. Introduction

The introduction of Bose gases and the prediction of Bose-Einstein condensates goes back to S. N. Bose [6] and A. Einstein [11] almost one century ago. By condensation we mean macroscopic occupation of a single particle state. In sharp contrast to bosons, this is not possible for identical fermions; a fact known as the Pauli exclusion principle. One of the reasons why Bose-Einstein condensation is interesting, lies in its connection to liquid Helium and its superfluidity. N. N. Bogolubov[1] attempted to explain this connection in his seminal paper from 1947 [5]. Since Bose-Einstein condensation only occurs in gases at very low temperatures and low density, several cooling methods had to be developed and then combined to create Bose-Einstein condensates in the laboratory. This experimental breakthrough happened in 1995, more than 70 years after Einstein's prediction. Experiments by the groups of E. A. Cornell and C. E. Wiemann confirmed the existence of Bose-Einstein condensates. Independently W. Ketterle produced a Bose-Einstein condensate in a slightly different set-up. The experiments, performed at around 20 nK were honoured with the Nobel Prize in 2001 [36]. Already at that time more than 20 groups had managed to produce Bose-Einstein condensates and the experimental interest intensified. At the time of writing this thesis, a search for "Bose-Einstein" has yielded more than 20.000 publications[2].

As one can read in [2], condensates have been created for a wide range of vapors with typical sizes between 1.5×10^3 and 10^6 atoms. Possibly inspired by the experimental success, there has also been an increase in theoretical work on Bose gases in the last decades. We refer to [25] for an overview of the mathematical work on the Bose gas and to [38, 39] for a physics point of view.

In this thesis we will restrict our interest to only one of the most fundamental quantities of a Bose gas – the ground state energy. More specifically:

How does the ground state energy of a dilute Bose gas at zero temperature depend on the density?

An answer to this question is essentially contained in Bogolubov's approximation and known as the Lee–Huang–Yang formula [21, 22], which describes the low density asymptotics of the ground state energy per volume in the thermodynamic limit, $e_0(\rho)$. The core of Bogolubov's theory is a very fruitful but non-rigorous diagonalization of the Hamiltonian. We will discuss Bogolubov's approximation step, which is well-motivated by the physics involved. One of the insights of Bogolubov is that the ground state energy

[1] Note that "Bogolubov" is not the only transliteration, which is used in the literature.

[2] The publication database webofknowledge.com was used with the search term "Bose-Einstein" on the 27.10.2017.

only depends on the potential via the scattering length, a. Our aim is to show that the Lee–Huang–Yang formula, which reads

$$e_0(\rho) = 4\pi\nu\rho^2 a \left(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}} + o(\sqrt{\rho a^3})\right) \qquad \text{as } \rho a^3 \to 0, \tag{1.1}$$

with $\nu = \frac{\hbar^2}{2m}$, is correct as a lower bound. To succeed, we will of course have to pose some restrictions on the class of potentials. Also we have to introduce an additional scaling to obtain our result. Concerning the rigorous proof of the lower bound, this is the second step forward towards establishing (1.1).

This is not merely a theoretical result, however. In experiments by Navon et al. [34, 35] the LHY-constant has been measured by changing the scattering length using Feshbach resonances. The measurements, 4.4(5), respectively 4.5(7), were in agreement with the predicted value $\frac{128}{15\sqrt{\pi}} \approx 4.81$. Also the Monte Carlo computations in [15] match the theoretical prediction well, if the LHY-correction term is included.

We end this introduction with an overview of the further sections in the present thesis: In Section 2, the background chapter, we fix notation and present mathematical background needed to formalize the description of the dilute Bose gas. The Hamiltonian for the system is introduced in position space and rewritten in second quantized form. This expression gives a heuristic argument for the leading order term of the ground state energy.
In Section 3 we present a calculation for the second order correction term (LHY-term) using the concept of c-number substitution, which is based on a condensation hypothesis, is used. This calculation invokes an approximation of the scattering length of the potential and can therefore only be correct in a certain scaling limit.
In Section 4 related mathematical literature on ground state energies for dilute Bose gases is reviewed.
In Section 5 we state the main result of this thesis:

For a broad range of potentials the LHY formula is correct as a lower bound for the ground state energy of a dilute Bose gas in a scaling regime, which goes beyond the mean inter-particle distance.

We present key ingredients leading to the proof of this statement. Furthermore, we point out some technical difficulties, which are responsible for the assumptions in our main theorem and conclude with remarks on possible improvements in future work.
Part II consists of the manuscript containing the mathematical proof for the mentioned result. This is an improvement compared to the work by Giuliani and Seiringer [17], who gave the until now only available proof for a lower bound capturing the second order correction.

2. Background

This section provides some background for the mathematical treatment of the Bose gas. Relevant length scales associated to gas are discussed and the corresponding many body Hamiltonian is rewritten in second quantized form using creation and annihilation operators. This standard bookkeeping method is then used to describe Bogolubov's c-number substitution and how it leads to the prediction that the ground state energy in the dilute limit is given by (1.1). This section is based on [25] and [44]. For additional background material the reader is referred to [12, 26, 42] and [43].

We consider a gas of N interacting particles. Particles in a interacting gas may be subject to both an external potential, e.g. some trap, which confines the gas to a region in space and an interaction-potential. Such a gas can be modelled by the Hamiltonian

$$H_N = \sum_{i=1}^{N} (-\Delta_i + V_{\text{ext},i}) + V_{\text{int}}, \tag{2.1}$$

which acts on the space $L^2(\mathbb{R}^{3N})$, i.e., the Hilbert space of square-integrable functions on $\mathbb{R}^{3N}$. We use the convention $\langle f, g\rangle := \int \overline{f}(x)g(x)\,\mathrm{d}x$ for the inner product of the functions $f, g \in L^2(\mathbb{R}^{3N})$. Here $\Delta_i f = \sum_{j=1}^{3} \frac{\partial^2 f}{\partial x_j^2}$, with $x_i = (x_1, x_2, x_3) \in \mathbb{R}^3$, is the Laplacian acting on the i^{th} particle. All Hilbert spaces that we will encounter in this thesis are going to be separable and infinite dimensional. Vectors of length unity play a special role. If $||\psi||_2 = 1$, we call ψ a wave function and interpret the quantity

$$|\psi(x_1, x_2, \ldots, x_N)|^2 \tag{2.2}$$

as the probability density for finding particle 1 at x_1, particle 2 at x_2 etc. Measurements correspond to self-adjoint operators. If the measurement corresponds to the (possibly unbounded) self-adjoint operator $\mathcal{A}$ and is performed on the state ψ, then

$$\langle \mathcal{A}\rangle_\psi := \langle \psi, \mathcal{A}\psi\rangle \tag{2.3}$$

is the expectation value for the measurement. The possible outcomes for a measurement are the elements in the spectrum of $\mathcal{A}$

$$\text{spec}\,(\mathcal{A}) := \{\lambda \in \mathbb{C} : (\mathcal{A} - \lambda \mathbb{1}) \text{ has no bounded inverse}\}\,, \tag{2.4}$$

which is contained in $\mathbb{R}$ if the operator is self-adjoint. Note that we in (2.3) do not have to require $\psi \in D\,(\mathcal{A})$, but only that ψ is contained in the domain of the quadratic form corresponding to $\mathcal{A}$. We only consider gases of identical bosons and these satisfy, by definition, the symmetry condition

$$\psi(x_1, x_2, \ldots, x_N) = \psi(x_{\sigma_1}, x_{\sigma_2}, \ldots, x_{\sigma_N}) \tag{2.5}$$

for any permutation $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ in the permutation group S_N of N elements[3]. Henceforth we will only consider Bose gases constrained to some box, say $\Lambda = [-\frac{L}{2}, \frac{L}{2}]^3$,

[3]For systems in two spacial dimensions interchanging two identical particles can give a phase other than ± 1, which shows that particle species other than fermions and bosons exist. Such particles are called *anyons* – a term coined by Frank Wilczek [46] – reflecting that indeed the "interchange of two of these particles can give *any* phase."

with side length $L > 0$. Instead of setting

$$V_{\text{ext}}(x) = \begin{cases} 0 & \text{if } x \in \Lambda \\ \infty & \text{if } x \notin \Lambda, \end{cases} \tag{2.6}$$

we simply drop the external potential and restrict our interest to the Hilbert space of permutation symmetric functions in $L^2(\Lambda)$ with Dirichlet boundary conditions. We then have

$$H_N = -\nu \sum_{i=1}^{N} \Delta_i + \sum_{1 \le i < j \le N} V(|x_i - x_j|), \tag{2.7}$$

with $\nu = \frac{\hbar^2}{2m}$, where m is the mass of a particle and $\hbar$ denotes the reduced Planck's constant. The *density* of a gas is defined by the number of particles per volume

$$\rho = \frac{N}{|\Lambda|}. \tag{2.8}$$

For notational convenience, we henceforth choose units such that $\nu = \hbar^2/(2m) = 1$.

2.1. Ground States and Grounds State Energies

The *ground state energy* of N interacting particles in the box $\Lambda = [-\frac{L}{2}, \frac{L}{2}]^3$ is

$$E_0(N, L) := \inf_{\substack{\Psi \in Q(H_N) \\ ||\Psi||=1}} \langle \Psi, H_N \Psi \rangle = \inf \operatorname{spec}(H_N), \tag{2.9}$$

where $Q(H_N)$ is the domain of the quadratic form corresponding to H_N. Note that the infimum in (2.9) not necessarily has to be attained or to be finite. In case $E_0(N, L)$ is finite, then the N-body system is called *stable*. We call ψ a *ground state* if it satisfies $\langle \psi, H_N \psi \rangle = E_0(N, L)$ and it can be shown that ψ is a ground state if and only if ψ is a solution to the Schrödinger equation $H_N \psi = E_0(N, L)\psi$. Our primary interest is to find a new second order lower bound for the energy per unit volume in the thermodynamic limit,[4]

$$e_0(\rho) := \lim_{\substack{N, L \to \infty \\ N/L^3 = \rho}} E_0(N, L) L^{-3}. \tag{2.10}$$

To obtain a heuristic understanding of the problem at hand, it is useful to consider which *length scales* are relevant. These are:

- a: the scattering length,
- $(\rho a)^{-\frac{1}{2}}$: the correlation length[5],
- $\rho^{-\frac{1}{3}}$: the mean inter-particle distance.

While the mean inter-particle distance simply is the order of the average distance to the next particle, the other two length scales require some explanation.

The correlation length can be understood in the following way. If the particles are localized to boxes of side length λ_c, then the uncertainty principle gives an energy of

[4] In Part II we use the less restrictive requirement $N, L \to \infty$ with $\lim_{N,L\to\infty} NL^{-3} = \rho$.

[5] This length scale is also known as the *uncertainty principle length*, *healing length*, *de Broglie wavelength* or the *Bogolubov length*.

order λ_c^{-2}. The energy per volume is then at least $N\lambda_c^{-2}L^{-3} = \rho\lambda_c^{-2}$, which is comparable to the leading order term $4\pi a\rho^2$ in (1.1) if $\lambda_c = \frac{1}{\sqrt{\rho a}}$.

We will see below that the *scattering length* a is a constant depending on the potential at hand. Since we are interested in the dilute limit, we have $\rho a^3 \ll 1$. In particular, we have $\rho^{-\frac{1}{3}} \ll \frac{1}{\sqrt{\rho a}}$. Hence, for states close to the ground state, we can only localize particles to boxes which are much larger than the mean inter-particle distance, showing that the wave functions overlap considerably for low densities.

2.2. The Scattering Length

We follow [25] and define the scattering length, which is a measure for the effective interaction strength of a potential. For simplicity we assume that $W \geq 0$, that W is spherically symmetric and that $W(x) = 0$ if $|x| > R_0$ for some R_0. These assumptions are less restrictive than those we have in Part II. In fact, the first and the third assumption can be relaxed [25].

The boundary of the ball B_R is denoted S_R and has surface area $4\pi R^2$. To discuss the two-body problem, we define on $\left\{\phi \in H^1(B_R) : \phi(x) = 1 \text{ for } x \in S_R\right\}$, where $R > R_0$, the map $\mathcal{E}_R$ by

$$\mathcal{E}_R[\phi] = \int_{B_R} |\nabla\phi(x)|^2 + \frac{1}{2}W(x)|\phi(x)|^2 \,\mathrm{d}x. \tag{2.11}$$

One can show that $\mathcal{E}_R$ has a unique minimizer, $0 \leq \phi_0 \leq 1$, which is spherically symmetric and radially increasing. Equation (2.11) is related to the zero-energy scattering equation

$$-\Delta\phi_0(x) + \frac{1}{2}W(x)\phi_0(x) = 0. \tag{2.12}$$

That this equation holds in the sense of distributions on B_R follows from the following standard computation [25]. Let $\psi \in C_0^\infty(B_R)$ and note that

$$\mathcal{E}_R[\phi_0 + \delta\psi] = \mathcal{E}_R[\phi_0] + \delta^2\mathcal{E}_R[\psi] + 2\delta\mathrm{Re}\int_{B_R} \nabla\phi_0 \cdot \nabla\psi + \frac{1}{2}W\phi_0\psi \,\mathrm{d}x. \tag{2.13}$$

Because ϕ_0 is a minimizer for $\mathcal{E}_R$, integration by parts yields

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}\delta}\mathcal{E}_R[\phi_0 + \delta\psi]_{|\delta=0} &= 2\mathrm{Re}\int_{B_R} \nabla\phi_0 \cdot \nabla\psi + \frac{1}{2}W\phi_0\psi \,\mathrm{d}x \\ &= 2\mathrm{Re}\int_{B_R} \psi\left[-\Delta\phi_0 + \frac{1}{2}W\phi_0\right]\mathrm{d}x + \int_{S_R} \psi\nabla\phi_0 \cdot \mathrm{d}S. \end{aligned} \tag{2.14}$$

The last term in (2.14) vanishes because $\psi \in C_0^\infty(B_R)$ and the claim follows by repeating the argument with ψ replaced by $i\psi$. An other way to state the above is that we employ the the Euler-Lagrange equation.

On the annulus $\mathcal{A}_{R_0,R} := \left\{x \in \mathbb{R}^3 : R_0 < |x| < R\right\}$ the scattering equation reduces to the requirement that ϕ_0 is harmonic. Combining this with the boundary condition $\phi(x) = 1$ for $x \in S_R$, we obtain on $\mathcal{A}_{R_0,R}$ that

$$\phi_0(x) = \frac{1 - \frac{a}{|x|}}{1 - \frac{a}{R}}, \qquad a \in [0, R_0]. \tag{2.15}$$

The constant a is called the *scattering length* and is determined by the value of ϕ_0 on S_{R_0}, i.e., the inner boundary of the above annulus, and depends on the potential through the scattering equation (2.12). The two examples below show that the scattering length indeed is a reasonable measure for the interaction range of the potential.

The minimum energy for $\mathcal{E}_R$ is found using the scattering equation (2.12) and integration by parts

$$\begin{aligned}\mathcal{E}_R[\phi_0] &= \int_{B_R} |\nabla\phi_0|^2 + \frac{1}{2}W|\phi_0|^2 \,\mathrm{d}x \\ &= \int_{S_R} \phi_0\nabla\phi_0 \cdot \mathrm{d}S + \int_{B_R} \phi_0 \left[-\Delta\phi_0 + \frac{1}{2}W(x)\phi_0\right] \mathrm{d}x \\ &= 4\pi a(1-\frac{a}{R})^{-1}. \end{aligned} \tag{2.16}$$

The leading order term $4\pi\rho^2 a$ in the LHY formula can, at least heuristically, be understood in the following way. The minimization problem (2.11) originates from the two-body problem via a center of mass integration such that ϕ_0 describes the relative position of the two particles. See [42] for an exposition. Because $\langle\phi_0, \phi_0\rangle$ is of order R^3 we make the ansatz

$$\lim_{R\to\infty} R^3 E_0(2,R) = 8\pi a. \tag{2.17}$$

We now obtain

$$e_0(\rho) = \lim_{\substack{N,R\to\infty \\ N/R^3=\rho}} E_0(N,R)R^{-3} \approx \lim_{\substack{N,R\to\infty \\ N/R^3=\rho}} 8\pi a\frac{N(N-1)}{2}R^{-6} = 4\pi\rho^2 a, \tag{2.18}$$

if we assume that energy is approximately linear in the number of pairs. This assumption neglects the interaction between the pairs. It is therefore reasonable, form the viewpoint of this heuristic description, that the second order correction term in the LHY formula is positive.

Example 1: For the hard-core potential with radius R_0, i.e.,

$$W_{R_0}(x) = \begin{cases} \infty & \text{if } |x| < R_0 \\ 0 & \text{if } |x| \geq R_0, \end{cases} \tag{2.19}$$

we have $\phi_0(x) = 0$ for $x \in B_{R_0}$ such that the scattering length agrees with the range of the potential; $a = R_0$.

Example 2: In the non-interacting case the scattering length vanishes. This is because $\phi_0 = \mathbb{1}_{B_R}$ if $W = 0$ and it then follows from (2.15) that $a = 0$.

The converse is also true. If $a = 0$, we have by (2.15) that $\phi_0 = 1$ on $\mathcal{A}_{R_0,R}$. The function ϕ_0 is subharmonic on B_R since W is positive. Because ϕ_0 attains its maximum on the interior of B_R, it follows from the maximum principle that ϕ_0 is constant. Thus $\phi_0 = \mathbb{1}_{B_R}$, and consequently $0 = \mathcal{E}_R(\mathbb{1}_{B_R}) = \int W = 0$. From the positivity of W we obtain $W = 0$.

For these two extreme examples we easily found values for the scattering length which make sense from a physics point of view. A natural question is:

Does the scattering length increase as the potential increases?

The answer is yes. Here we give a modified version of the proof of Lemma C.3 in [25], where it is proven using contradiction.

Let (V, ϕ_0, a) and $(\widetilde{V}, \widetilde{\phi}_0, \widetilde{a})$ be triples consisting of potential, scattering solution and scattering length satisfying $V \geq \widetilde{V} \geq 0$. Then we have $a \geq \widetilde{a}$.

It follows from the scattering equation (2.12) that the difference of the scattering solutions, $g := \phi_0 - \widetilde{\phi}_0$, is subharmonic. Hence g attains its maximum on S_R. Since $\phi_0(x) = \widetilde{\phi}_0(x) = 1$ for $x \in S_R$, we have $\phi_0 \geq \widetilde{\phi}_0$ and therefore $a \geq \widetilde{a}$.

2.3. Fock Space

We now introduce Fock space [14], which is a standard technical tool and allows one to deal with variable particle numbers. Given a Hilbert space $\mathcal{H}$, we define $\mathcal{H}_0 = \mathbb{C}$, $\mathcal{H}_1 = \mathcal{H}$ and $\mathcal{H}_N = \mathcal{H}_{N-1} \otimes \mathcal{H}$ for $N > 1$. On $\mathcal{H}_N$ we define the orthogonal projections

$$P_N^+ \left(\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_N\right) = \sum_{\sigma \in S_N} \frac{1}{N!} \psi_{\sigma_1} \otimes \psi_{\sigma_2} \otimes \cdots \otimes \psi_{\sigma_N}, \tag{2.20}$$

$$P_N^- \left(\psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_N\right) = \sum_{\sigma \in S_N} \frac{(-1)^{|\sigma|}}{N!} \psi_{\sigma_1} \otimes \psi_{\sigma_2} \otimes \cdots \otimes \psi_{\sigma_N}, \tag{2.21}$$

where $|\sigma|$ is the order of the permutation $\sigma \in S_N$. The *Fock space* is the Hilbert space

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N. \tag{2.22}$$

Using the projections in (2.20), respectively (2.21), we define the bosonic, respectively fermionic, Fock spaces

$$\mathcal{F}_+ = \bigoplus_{N=0}^{\infty} \bigotimes_{\substack{i=1 \\ \text{sym}}}^{N} \mathcal{H} := \bigoplus_{N=0}^{\infty} \bigotimes^{N} P_N^+ \left(\mathcal{H}_N\right), \tag{2.23}$$

$$\mathcal{F}_- = \bigoplus_{N=0}^{\infty} \bigwedge_{i=1}^{N} \mathcal{H} := \bigoplus_{N=0}^{\infty} \bigotimes^{N} P_N^- \left(\mathcal{H}_N\right). \tag{2.24}$$

The vector $|\Omega\rangle = 1 \in \mathbb{C}$ plays a special role and is often called the vacuum. Sometimes it is convenient to specify a state, i.e., a normalized vector in $\mathcal{F}$ by letting creation and annihilation operators act on the vacuum state. By linearity it suffices to define how the annihilation operator, $a(f)$, maps pure tensors in the N-particle sector $\mathcal{H}_N$ into $\mathcal{H}_{N-1}$ and the creation operator, $a^*(f) := (a(f))^*$, maps pure tensors in $\mathcal{H}_N$ into $\mathcal{H}_{N+1}$

$$a(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_N) = N^{\frac{1}{2}} \langle f | f_1 \rangle f_2 \otimes f_3 \otimes \cdots \otimes f_N, \tag{2.25}$$

$$a^*(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_N) = (N+1)^{\frac{1}{2}} f \otimes f_1 \otimes \cdots \otimes f_N. \tag{2.26}$$

We then have that $\mathcal{H} \ni f \mapsto a^*(f)$ is linear and that $f \mapsto a(f)$ is anti-linear. Note that the restriction of $a(f)$, respectively $a^*(f)$, to any N-particle sector defines a bounded operator, while $a(f)$ is an unbounded operator defined on the domain

$$\left\{ \psi = \bigoplus_{N=0}^{\infty} \psi_N \Big| \sum_{N=0}^{\infty} N ||\psi_N||^2 < \infty \right\}. \tag{2.27}$$

We also note that the operators $a(f)$ preserve symmetry, respectively anti-symmetry; but that the operators $a(f)^*$ do not. That is

$$\psi \in \mathcal{F}_\pm \nRightarrow a(f)^*\psi \in \mathcal{F}_\pm. \tag{2.28}$$

When working on the bosonic/fermionic Fock space, $\mathcal{F}_\pm$, this problem is circumvented by projecting down onto $\mathcal{F}_\pm$ after applying $a(f)^*$.

2.1. DEFINITION (Bosonic and fermionic creation operator)**.**
For $f \in \mathcal{H}$, we define the bosonic and fermionic creation operator by

$$a_\pm(f)^* = P_\pm\left(a(f)^*\right). \tag{2.29}$$

Given an operator h on $\mathcal{H}$, we will let h_i denote the operator acting on the i^{th} copy of $\mathcal{H}$ in the N-particle sector $\mathcal{H}_N = \bigotimes_{i=1}^{N} \mathcal{H}$, i.e.,

$$h_i = \mathbb{1}_\mathcal{H} \otimes \cdots \otimes \mathbb{1}_\mathcal{H} \otimes \underset{i^{\text{th}}\ \text{factor}}{h} \otimes \mathbb{1}_\mathcal{H} \otimes \cdots \otimes \mathbb{1}_\mathcal{H} \tag{2.30}$$

and define on $\mathcal{F}$ the second quantization of the one-particle operator h by

$$\Gamma(h) := \bigoplus_{N=1}^{\infty} \sum_{i=1}^{N} h_i. \tag{2.31}$$

If the Hamiltonian describing our system would only contain terms of the form (2.31), there would be no interaction between the particles. Finding the ground state energy for the N-particle Hamiltonian would then not be harder than finding the ground state energy for the one-particle Hamiltonian. The difficulty in dealing with a Hamiltonian of the form (2.7) therefore really comes from the interaction *between* the particles.

3. Aspects of Bogolubov Theory

In this section we will consider particles in the box $\Lambda = [-\frac{L}{2}, \frac{L}{2}]^3$ with periodic boundary conditions. While this boundary condition is somewhat unphysical, it is the preferred because it allows us to use the orthonormal basis

$$\left\{ u_p(x) = L^{-\frac{3}{2}} e^{ipx} \mid p \in \Lambda^* \right\}, \tag{3.1}$$

for $\mathcal{H} = L^2(\Lambda)$, where $\Lambda^* := (\frac{2\pi}{L})\mathbb{Z}^3$. It is standard to rewrite the Hamiltonian introduced in (2.7) in second quantized form using creation and annihilation operators. Using the bosonic creation operator a_+^*, defined in (2.29), we define $a_p : \mathcal{F}_+(\mathcal{H}) \to \mathcal{F}_+(\mathcal{H})$ by

$$a_p\psi = a_+(u_p)\psi \qquad \text{and} \qquad a_p^*\psi = a_+(u_p)^*\psi. \tag{3.2}$$

The bosonic creation and annihilation operators satisfy the *Canonical Commutation Relation* (CCR)

$$\forall p, q \in \Lambda^* : \qquad [a_p, a_q] = \left[a_p^*, a_q^*\right] = 0 \qquad \text{and} \qquad \left[a_p, a_q^*\right] = \delta_{p,q}\mathbb{1}, \tag{3.3}$$

where $[A, B] = AB - BA$ denotes the commutator of A and B.

Given a symmetric operator h on $\mathcal{H}$, we can write its second quantization as

$$\Gamma(h) = \sum_{p,q\in\Lambda^*} \langle u_p, h u_q\rangle a_p^* a_q = \sum_{p,q\in\Lambda^*} h_{p,q} a_p^* a_q, \tag{3.4}$$

where we have defined $h_{p,q} = \langle u_p, h u_q\rangle$, considered the action of $\Gamma(h)$ on pure states in the N-particle sectors and expanded in the basis $\{u_p \mid p \in \Lambda^*\}$ (see Lem. 7.8, [44]). In particular, the second quantization of the identity is

$$\Gamma(\mathbb{1}) = \sum_{p,q\in\Lambda^*} \delta_{p,q} a_p^* a_q = \sum_{p\in\Lambda^*} a_p^* a_p = \bigoplus_{N=0}^{\infty} N \mathbb{1}_{\mathcal{H}_N^+} =: \mathcal{N}, \tag{3.5}$$

which is the *number operator*. There are two more number operators which play an important role in our analysis. With $\Lambda_+^* := \Lambda^* \backslash \{0\}$ these are

$$\mathcal{N}_+ := \sum_{p\in\Lambda_+^*} a_p^* a_p, \tag{3.6}$$

which counts the amount of excited particles, and

$$\mathcal{N}_0 := a_0^* a_0, \tag{3.7}$$

which counts the amount of particles in the condensate. The second quantized Laplacian is given by

$$\Gamma(-\Delta) = \sum_{p\in\Lambda^*} p^2 a_p^* a_p. \tag{3.8}$$

For the Fourier transform we use the convention

$$(\mathcal{F}\psi)(k) = \widehat{\psi}(k) = \int \psi(x) e^{-ikx}\, \mathrm{d}x. \tag{3.9}$$

We call W a 2-body potential if $W : \mathcal{H} \otimes \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$ is symmetric and for all $(a \otimes b) \in \mathcal{H} \otimes \mathcal{H}$ satisfies

$$W(a \otimes b) = W(b \otimes a). \tag{3.10}$$

Similar to (3.4) we can second quantize W by setting

$$\Gamma(W) = \sum_{p,q,r,s\in\Lambda^*} \langle u_r \otimes u_s, W u_p \otimes u_q\rangle a_r^* a_s^* a_p a_q = \sum_{p,q,r,s\in\Lambda^*} W_{rspq} a_r^* a_s^* a_p a_q, \tag{3.11}$$

where we have defined $W_{rspq} = \langle u_r \otimes u_s, W u_p \otimes u_q\rangle$. If we define the periodization of the potential W by

$$W_{\mathrm{Per}}(x) := \frac{1}{|\Lambda|} \sum_{k\in\Lambda^*} \widehat{W}(k) e^{ikx}, \tag{3.12}$$

we see that

$$\begin{aligned}\langle u_r \otimes u_s, W_{\mathrm{Per}}(x-y)u_p \otimes u_q\rangle &= \langle u_r \otimes u_s, \frac{1}{|\Lambda|}\sum_{k\in\Lambda^*}\widehat{W}(k)e^{ik(x-y)}u_p \otimes u_q\rangle \\ &= \frac{1}{|\Lambda|}\sum_{k\in\Lambda^*}\widehat{W}(k)\delta_{r,p+k}\delta_{s,q-k}. \end{aligned} \tag{3.13}$$

Inserting this into (3.11), we obtain

$$\Gamma\left(W_{\mathrm{Per}}\right) = \frac{1}{|\Lambda|}\sum_{p,q,k\in\Lambda^*}\widehat{W}(k)a^*_{p+k}a^*_{q-k}a_pa_q. \tag{3.14}$$

There are $\frac{N(N-1)}{2}$ pairs of particles and we may therefore replace the Hamiltonian in (2.7) with

$$\sum_{k\in\Lambda^*}k^2a^*_ka_k + \frac{1}{2|\Lambda|}\sum_{p,q,k\in\Lambda^*}\widehat{W}(k)a^*_{p+k}a^*_{q-k}a_pa_q. \tag{3.15}$$

We collect terms in (3.15) with $k=0$ and obtain

$$\begin{aligned}&\sum_{k\in\Lambda^*}k^2a^*_ka_k + \frac{1}{2|\Lambda|}\sum_{p,q\in\Lambda^*}\widehat{W}(0)a^*_pa^*_qa_pa_q + \sum_{k\in\Lambda^*_+}\frac{1}{2|\Lambda|}\sum_{p,q\in\Lambda^*}\widehat{W}(k)a^*_{p+k}a^*_{q-k}a_pa_q \\ =&\sum_{k\in\Lambda^*}k^2a^*_ka_k + \frac{(N-1)}{2}\rho\widehat{W}(0) + \sum_{k\in\Lambda^*_+}\frac{1}{2|\Lambda|}\sum_{p,q\in\Lambda^*}\widehat{W}(k)a^*_{p+k}a^*_{q-k}a_pa_q, \end{aligned} \tag{3.16}$$

where we have used that $\rho = \frac{N}{|\Lambda|}$. The next step is to group the third term in (3.16) according to the number of $a^\sharp_0$'s, where $a^\sharp_0$ is either a_0 or a^*_0 and to simply cancel terms with only one $a^\sharp_0$ or no $a^\sharp_0$ at all. We have:

4-$a^\sharp_0$: No contribution - would imply $k=0$,
3-$a^\sharp_0$: No contribution - momentum conservation,
2-$a^\sharp_0$: $\frac{1}{2|\Lambda|}\sum_{k\in\Lambda^*_+}\widehat{W}(k)\left[a^*_0a^*_0a_{-k}a_k + a^*_ka^*_{-k}a_0a_0 + a^*_0a^*_ka_ka_0 + a^*_ka^*_0a_0a_k\right]$,
1-$a^\sharp_0$: Neglected,
0-$a^\sharp_0$: Neglected.

The rationale behind this idea is that if the gas is sufficiently dilute and the interaction therefore weak, then the ground state of the interacting gas should be *close* to the ground state for the non-interacting gas, i.e., $\psi_0\otimes\cdots\otimes\psi_0$. This argument is called the *condensation hypothesis*. In particular it is reasonable to assume that in the thermodynamic limit $N=\langle a^*_0a\rangle$ to first order and hence that $\langle n_+\rangle \ll N$. We therefore substitute $a^\sharp_0 = \sqrt{N} = \sqrt{\rho|\Lambda|}$ and neglect terms with three or more terms of the form $a^\sharp_k$. We have now arrived at the Hamiltonian

$$\sum_{k\in\Lambda^*}k^2a^*_ka_k + \frac{(N-1)}{2}\rho\widehat{W}(0) + \frac{\rho}{2}\sum_{k\in\Lambda^*_+}\widehat{W}(k)\left[a_{-k}a_k + a^*_ka^*_{-k} + a^*_ka_k + a^*_ka_k\right] \tag{3.17}$$

$$= \frac{(N-1)}{2}\rho\widehat{W}(0) + \sum_{k\in\Lambda^*_+}(\frac{k^2}{2} + \frac{\rho}{2}\widehat{W}(k))(a^*_ka_k + a^*_{-k}a_{-k}) + \frac{\rho}{2}\widehat{W}(k)\left(a^*_{-k}a^*_k + a_ka_{-k}\right), \tag{3.18}$$

where we have used that $\widehat{W}$ is even. Note that this Hamiltonian is quadratic in $a_k^\sharp$. The advantage of quadratic Hamiltonians is that they under reasonable assumptions can be diagonalized using Bogolubov transformations. A lower bound for this Hamiltonian (3.18) can be found using the following theorem, which follows from (Thm. 6.3, [27]) by setting $\kappa = 0$ and replacing $b_\pm$ by $\pm i b_\pm$.

3.1. THEOREM (Simple case of Bogolubov's method)**.**
For $\mathcal{A}, \mathcal{B} \in \mathbb{R}$ satisfying $\mathcal{A} \geq 0$ and $-\mathcal{A} \leq \mathcal{B} \leq \mathcal{A}$ we have the operator inequality

$$\mathcal{A}(b_+^* b_+ + b_-^* b_-) + \mathcal{B}(b_+^* b_-^* + b_+ b_-) \geq -\tfrac{1}{2}(\mathcal{A} - \sqrt{\mathcal{A}^2 - \mathcal{B}^2})([b_+, b_+^*] + [b_-, b_-^*]),$$

where $b_\pm$ are operators on a Hilbert space satisfying $[b_+, b_-] = 0$.

For all $p \in \Lambda^*$ we apply the theorem with

$$b_+ = a_k, \qquad b_- = a_{-k}, \qquad \mathcal{A} = \frac{k^2}{2} + \frac{\rho\widehat{W}(k)}{2} \qquad \text{and} \qquad \mathcal{B} = \frac{\rho\widehat{W}(k)}{2}. \tag{3.19}$$

We obtain

$$\begin{aligned} &\sum_{k \in \Lambda_+^*} (\frac{k^2}{2} + \rho\widehat{W}(k))(a_k^* a_k + a_{-k}^* a_{-k}) + \widehat{W}(k)\left(a_{-k} a_k + a_{-k}^* a_k^*\right) \\ &\geq \sum_{k \in \Lambda_+^*} -\frac{1}{2}\left(k^2 + \rho\widehat{W}(k) - \sqrt{k^4 + 2\rho\widehat{W}(k)k^2}\right). \end{aligned} \tag{3.20}$$

The last step towards the LHY formula is to employ the Born series for a potential W, which we in Part II define as

$$\sum_{k=1}^{\infty} a_k(W) := (8\pi)^{-1} \int_{\mathbb{R}^3} W(x)\,\mathrm{d}x - \sum_{k=2}^{\infty} (-8\pi)^{-k} \int_{\mathbb{R}^3} (\mathcal{L}_W)^{k-1}(W)(x)\,\mathrm{d}x\,, \tag{3.21}$$

where $\mathcal{L}_W$ is the operator given by $\mathcal{L}_W(g)(x) = W(x)\int_{\mathbb{R}^3} |x-y|^{-1} g(y)\,\mathrm{d}y$. If (3.21) converges, it yields the scattering length. The expansion provides the starting point for simplifying the Hamiltonian in a mathematically rigorous way. The interaction potential W is replaced by a rescaled version

$$W_R(x) := \frac{1}{R^3} W(R^{-1}x), \tag{3.22}$$

where $R \gg a$ is a scaling parameter. Comparing the Born series for these potential, we see that $a_k(W_R)$ scales with $\left(\frac{a}{R}\right)^{k-1}$ and, in particular, that we have

$$a_1(W) = \int W\,\mathrm{d}x = \int W_R\,\mathrm{d}x = a_1(W_R) = a(W_R) + O(R^{-1}). \tag{3.23}$$

The sum is replaced by an integral in passing to the thermodynamic limit. Furthermore we add and subtract a term corresponding to the second Born approximation to the scattering length

$$\begin{aligned} e_0(\rho) \geq{}& \frac{\rho^2\widehat{W}(0)}{2} - \frac{1}{4}(2\pi)^{-3}\rho^2 \int_{\mathbb{R}^3} \frac{\widehat{W}(k)^2}{k^2}\,\mathrm{d}k \\ &- \frac{1}{2}(2\pi)^{-3} \int_{\mathbb{R}^3} k^2 \left(1 + \frac{\rho\widehat{W}(k)}{k^2} - \frac{\rho^2\widehat{W}(k)^2}{2k^4} - \sqrt{1 + \frac{2\rho\widehat{W}(k)}{k^2}}\right)\mathrm{d}k. \end{aligned} \tag{3.24}$$

Expanding the square root, we see that the integrand is bounded by Ck^{-2} for small $|k|$ and bounded by Ck^{-4} for large $|k|$ and therefore that the integral is convergent. From the identities

$$a_1 = (8\pi)^{-1}\widehat{W}(0) \qquad \text{and} \qquad a_2 = -\frac{1}{128\pi^4}\int_{\mathbb{R}^3}\frac{\widehat{W}(k)^2}{k^2}\,\mathrm{d}k \tag{3.25}$$

we get

$$e_0(\rho) \geq 4\pi\rho^2\left(a_1 + a_2\right) - \frac{1}{2}(2\pi)^{-3}\int_{\mathbb{R}^3} k^2\left(1 + \frac{\rho\widehat{W}(k)}{k^2} - \frac{\rho^2\widehat{W}(k)^2}{2k^4} - \sqrt{1 + \frac{2\rho\widehat{W}(k)}{k^2}}\right)\mathrm{d}k. \tag{3.26}$$

With the substitution $k \mapsto \sqrt{\rho\widehat{W}(0)}k$, dominated convergence and the identity

$$-\int_{\mathbb{R}^3} k^2 + 1 - k^2\sqrt{1 + 2k^{-2}} - \frac{1}{2k^2}\,\mathrm{d}k = \frac{32}{15}\pi\sqrt{2} \tag{3.27}$$

we obtain

$$e_0(\rho) \geq 4\pi\rho^2\left(a_1 + a_2 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\left(\sqrt{\rho a^3}\right)\right). \tag{3.28}$$

The sum $a_1 + a_2$ is the beginning of the Born series for the scattering length. If we now replace W by W_R, defined in (3.22), the scattering length for the rescaled potential satisfies

$$a = a_1 + O(R^{-1}) \tag{3.29}$$

and

$$a = a_1 + a_2 + O(R^{-2}). \tag{3.30}$$

In the regime $(\rho a^3)^{-\frac{1}{4}} \ll \frac{R}{a} \ll (\rho a^3)^{-\frac{1}{2}}$ we obtain the LHY formula

$$e_0(\rho) \geq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\left(\sqrt{\rho a^3}\right)\right) \tag{3.31}$$

as a lower bound.

4. Upper and Lower Bounds

In this section we briefly review former work on the ground state energy of dilute Bose gases. For a more detailed discussion the reader is referred to [25].
The basis for the bounds below was laid in Bogolubov's article [5], the importance of which we have already stressed. To discuss some of the previous bounds, we denote the thermodynamic limit of the ground state energy *per particle* by $\widetilde{e}_0(\rho)$.

Based on Bogolubov's work, Lee, Huang and Yang [21, 22] calculated in 1957 the asymptotic formula

$$\widetilde{e}_0(\rho) = 4\pi\rho a \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho a^3})\right), \tag{4.1}$$

using a generalization "of Fermi's pseudopotential" [19], which we do not discuss here. An upper bound for the leading order term $4\pi\rho a$ was proved in 1957 by Dyson [10] in the context of hard-core bosons. Dyson also provided a lower bound, which however was too small by a factor of $10\sqrt{2} \approx 14$. For hard-core bosons the energy is purely kinetic. A key idea in Dyson's proof was to sacrifice the kinetic energy in order to obtain a 'soft' potential with a potential energy component, which then could be analysed. The idea of sacrificing kinetic energy has been used in different forms in the following proofs for lower bounds on the asymptotics of the dilute Bose gas[6].

Possibly stimulated by the advances in experimental as well as theoretical physics, Lieb and Yngvason continued Dyson's work in [29] and refined the idea of sacrificing the kinetic energy and using Temple's inequality [45] on smaller boxes paving the thermodynamic box. By controlling the number of particles in each of the smaller boxes, it was obtained that

$$\widetilde{e}_0(\rho) \geq 4\pi\rho a \left(1 - C(\rho a^3)^{\frac{1}{17}}\right) \tag{4.2}$$

if the two-body potential is repulsive, spherically symmetric and has finite range. Recently J. O. Lee [20] showed that a similar bound to (4.2) – the exponent for the error term differs – also holds for a class of potentials, which is not repulsive. In [49] J. Yin showed that the lower bound (4.2) also holds for a similar class of non-repulsive potentials as studied in [20]. A rigorous verification of the Lee–Huang–Yang formula, including the second order correction term, was given by Giuliani and Seiringer in [17]. However, the proof relies on rescaled potentials[7] $v_R(x) = \frac{a_1}{R^3} v_1(x/R)$ and is therefore only valid in a certain scaling limit. The potential v_1 was chosen to be the periodized Yukawa potential, i.e., the periodization of $v_1(x) = e^{-|x|}$. For the lower bound it was required that $\frac{a}{R} = O((\rho a^3)^{\frac{1}{2}-d})$ with $0 < d < \frac{1}{69}$. In particular $\lim_{\rho\to 0} \rho^{\frac{1}{3}} R = \infty$ is needed, which explains the formulation "*weak coupling* and *high density* regime" in the paper. There are a couple of similarities between [17] and Part II. Both projects use the sliding argument from [7][8] with a background Hamiltonian, a priori and improved bounds for the number of particles, a lower bound on the respective quadratic parts via a version of Lemma 3.1 and the method of localizing large matrices [27] to show that $\langle n_+^2 \rangle$ and $\langle n_+ \rangle^2$ are similar for states close to the ground state. In [17] a variational state, which appeared earlier in [16], inspired by Bogolubov's approach, was used to provide an upper bound.

[6]A comment by Dyson on this paper can be found in the interview [37].
[7]Note that the rescaled potential in [17] (compare to (5.4)) contains the first Born term, which we here denote by a_1 instead of a_0.
[8]See also [28].

In [13] Erdős, Schlein and Yau give an upper bound for potentials of the form $V = \lambda\widetilde{V}$, where $\lambda > 0$ and $\widetilde{V}$ is a repulsive and sufficiently regular potential. Their upper bound

$$\widetilde{e}_0(\rho) \leq 4\pi\rho a \left[1 + \frac{128}{15\sqrt{\pi}} S_\lambda \sqrt{\rho a^3} + O(\rho a^3 |\ln \rho a^3|)\right] \tag{4.3}$$

with $S_\lambda \leq 1 + C\lambda$ gives the LHY formula in the additional limit $\lambda \to 0$. A similar result follows from [33].

The most recent upper bound, which also captures the second term in (4.1), is given in [48] for repulsive and sufficiently regular potentials. In contrast to [13] the variational state in [48] is more general and allows for so called *soft pairs*.

For results in other dimension than 3 we mention [1, 24, 30, 31, 40, 47]. In recent years a series of works going beyond the ground state energy and describing the excitation spectrum of the Bose gas has appeared [3, 4, 9, 18, 23, 32, 41]. For a review we refer to [43].

5. A New Lower Bound

The aim of this section is to give an overview of key ideas and techniques that have been used in Part II. We will reproduce some of the estimates, but avoid explicit error terms and instead only argue why the error-terms are small relative to the LHY-order. We would like to show that a Bose gas, described by the Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \leq i < j \leq N} v(|x_i - x_j|), \tag{5.1}$$

in the thermodynamic limit has a ground state energy per volume which is lower bounded by the LHY formula

$$e(\rho) \geq 4\pi\rho^2 a \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\left(\sqrt{\rho a^3}\right)\right) \qquad \text{as } \rho a^3 \to 0. \tag{5.2}$$

This formula is expected to hold for spherically symmetric potentials for which the scattering length is positive - including the hard-core potential. Furthermore (5.2) is expected to hold as an upper bound.

Unfortunately, proving (5.2) seems still to be beyond reach in full generality. By replacing the potential with a rescaled potential, we obtain a simpler problem which then can be solved. This approach has already been employed successfully in [17] to the problem that we are interested in. Over time one may hope to extend the scaling range for which the solution holds until rescaled potentials are no longer needed. From this point of view Part II can be seen as a new step forward in the quest of establishing a rigorous second order lower bound for the ground state energy of the dilute Bose gas.

We will now discuss the main ingredients for the proof in Part II. In our proof we introduce various length scales, which satisfy

$$a \ll R, \rho^{-1/3} \ll ds\ell \ll d\ell \ll (\rho a)^{-1/2} \ll s\ell \ll \ell. \tag{5.3}$$

The length scales $a, \rho^{-\frac{1}{3}}$ and $(\rho a)^{-\frac{1}{2}}$ are physical and have been discussed on page 12. Our first step is to simplify the problem by introducing rescaled potentials.

Rescaled potentials: The rescaled potential is defined as in (3.22) by

$$v_R(x) := \frac{1}{R^3} v_1(R^{-1}x). \tag{5.4}$$

All assumptions on the potential regarding regularity, respectively scaling, are collected in the two following conditions.

CONDITION 1: *We assume that v_1 is radially symmetric, non-negative, continuous, has compact support and satisfies $v_1(0) > 0$.*

The scaling range for R is defined via

CONDITION 2: *We require that*

$$\lim_{\rho \to 0} R\rho^{1/3}(\rho a^3)^{1/6} = 0 \tag{5.5}$$

and, for $\eta = \frac{1}{30}$,

$$\lim_{\rho \to 0} R\rho^{1/3}(\rho a^3)^{-\eta} = \infty. \tag{5.6}$$

The assumed compact support in Condition 1 can most likely be replaced by sufficiently fast decay. This would however require an even more technical proof. The condition in (5.5) corresponds to requiring that R has to be asymptotically smaller than the "uncertainty length" $\lambda_c = (\rho a)^{-\frac{1}{2}}$ and hence that a_2 is smaller than $(\rho a)^{-\frac{1}{2}}$.

The numerical value $\frac{1}{30} > 0$ arises from an estimate at the very end of Part II, where a portion of the kinetic energy is used to bound the $\mathcal{Q}_3$-term, which we introduce on page 27. Note that R here, in contrast to [17], is allowed (but not required) to be much smaller than the mean particle distance $\rho^{-\frac{1}{3}}$. The notation (5.5) and (5.6) has been chosen in Part II to stress this fact. This is also why we wrote that our proof works in a *weak coupling* ($\rho a^3 \ll 1$) and *low density* ($R \ll \rho^{-\frac{1}{3}}$) regime. More compactly, we write

$$(\rho a^3)^{-\frac{3}{10}} \ll \frac{R}{a} \ll (\rho a^3)^{-\frac{1}{2}}. \tag{5.7}$$

We can now state the simplified problem by redefining our Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \leq i < j \leq N} v_R(x_i - x_j). \tag{5.8}$$

Our main result is

5.1. THEOREM (Main theorem)**.** *Let H_N be defined as in (5.8) and assume that Conditions 1 and 2 are satisfied. The corresponding ground state energy per volume, $e(\rho)$, then satisfies*

$$e(\rho) \geq 4\pi\rho^2 a \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\left(\sqrt{\rho a^3}\right)\right) \qquad as \quad \rho a^3 \to 0. \tag{5.9}$$

The background Hamiltonian: The second idea in the proof is to introduce the background Hamiltonian

$$H_{\rho,N} = \sum_{j=1}^{N} \left(-\Delta_j - \rho \int v_R(x) \, \mathrm{d}x \right) + \sum_{1\le i<j\le N} v_R(x_i - x_j) + \frac{1}{2}\rho^2 |\Lambda| \int v_R(x) \, \mathrm{d}x. \tag{5.10}$$

The first and the third term in (5.10) are the original Hamiltonian, i.e., the kinetic part and the particle-particle interaction. The second term is the particle-background interaction, while the last term is the background-background interaction. For simplicity we have chosen the same density for the gas and the background. This is not optimal and should be changed if we want to extend our scaling range. For the present proof the difference is however negligible. The ground state energies for the background Hamiltonian, $e_0(\rho)$, respectively the usual Hamiltonian for the rescaled potential, $e(\rho)$, are related via

$$e(\rho) \ge e_0(\rho) + \lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} \rho \frac{N}{|\Lambda|} \int v_R - \frac{1}{2}\rho^2 \int v_R = e_0(\rho) + 4\pi\rho^2 a_1, \tag{5.11}$$

which can be seen using the ground state of H_N as a trial state for the background Hamiltonian. If $\frac{R}{a} \gg (\rho a^3)^{-\frac{1}{4}}$, we have from the Born approximation that
$a = a_1 + a_2 + O(\frac{1}{R^2}) = a_1 + a_2 + o(\sqrt{\rho a^3})$. Our requirement on R in Condition 2 is much stronger. Instead of proving the LHY formula (5.9) for the Hamiltonian (5.8) directly, we therefore focus on the Background Hamiltonian and show that its ground state energy satisfies

$$e_0(\rho) \ge 4\pi\rho^2 \left(a_2 + \frac{128}{15\sqrt{\pi}} a(\sqrt{\rho a^3} + o(\sqrt{\rho a^3})) \right) \qquad \text{as} \quad \rho a^3 \to 0, \tag{5.12}$$

which is the same approach that we outlined in Section 3.

5.1. Localization of the Background Hamiltonian

Our two-step localization procedure for the background Hamiltonian evolved from the localization method in [27], which is based on the localization in [7]. Since we want to prove a lower bound on the ground state energy, we use Neumann boundary conditions and boxes with side length $\ell \gg (\rho a^3)^{-\frac{1}{2}}$ such that the localization error is negligible. In fact, we do not stop here. We go one step further and localize one more time to a length scale which is smaller than $(\rho a^3)^{-\frac{1}{2}}$. On these smaller boxes the localization error is non-negligible. Using the small boxes, we will obtain an a priori estimate on the energy on the large boxes. This bound has the correct leading order term, but a second order term which has the wrong order. However, we can come reasonably close and use the bound that we obtain as the starting point for the estimates on the larger localization boxes.
Because of the Neumann boundary condition the lowest kinetic energy is now attained by the constant function, which we identify with the condensate. Particles orthogonal to the condensate are *excited*. If we have N particles in the thermodynamic box, we do not know how these are distributed over the localization boxes. This problem is resolved by showing that if the energy in a localization box is low, then the particle number can not deviate too much from the average. Arguments of this type give increasingly good

control over the number of particles, number of particles in the condensate and number of excited particles.

Localization of potential energy: To obtain localized Hamiltonians, we introduce the following boxes

$$B(u) = \ell\left([-\tfrac{1}{2},\tfrac{1}{2}]^3 + u\right), \quad \widetilde{B}(u') = d\ell\left([-\tfrac{1}{2},\tfrac{1}{2}]^3 + u'\right), \quad B(u,u') = B(u)\cap\widetilde{B}(u'), \tag{5.13}$$

where d and ℓ are parameters satisfying $d\ell \ll (\rho a)^{-\frac{1}{2}} \ll \ell$. For concreteness we chose the cut-off function

$$\chi(x) = \begin{cases} C_M\left(\cos(\pi x_1)\cos(\pi x_2)\cos(\pi x_3)\right)^{M+1} & \text{if } x\in[-\frac{1}{2},\frac{1}{2}]^3 \\ 0 & \text{if } x\notin[-\frac{1}{2},\frac{1}{2}]^3, \end{cases} \tag{5.14}$$

satisfying $0 \leq \chi \in C_0^M$, where M is a sufficiently large integer and C_M such that $||\chi||_2 = 1$. Letting

$$\chi_u(x) = \chi(\frac{x}{\ell} - u) \qquad \text{and} \qquad \widetilde{\chi}_{u'}(x) = \chi(\frac{x}{d\ell} - u'), \tag{5.15}$$

we obtain the localization function

$$\chi_B(x) = \begin{cases} \chi_u(x) & \text{if } B = B(u) \\ \chi_u(x)\widetilde{\chi}_{u'}(x) & \text{if } B = B(u,u'). \end{cases} \tag{5.16}$$

The rescaled potential can now be replaced by the localized potentials

$$\omega_{B(u)}(x,y) = \chi_{B(u)}(x)\frac{v_R(x-y)}{\chi*\chi((x-y)/\ell)}\chi_{B(u)}(y) \tag{5.17}$$

and

$$\omega_{B(u,u')}(x,y) = \chi_{B(u,u')}(x)\frac{v_R(x-y)}{\chi*\chi((x-y)/\ell)\chi*\chi((x-y)/(d\ell))}\chi_{B(u,u')}(y). \tag{5.18}$$

Indeed $\omega_B(x,y) \neq 0$ only if $x,y\in B$. Well-definedness of the localized potentials follows from the scaling $R \ll d\ell \ll \ell$, which we assumed in (5.3). Writing the convolution in symmetric form, i.e., $(\chi*\chi)(x-y) = \int\chi(x-u)\chi(y-u)\,\mathrm{d}u$, it is straight forward to show that

$$\chi*\chi((x-y)/\ell) = \int\chi_{B(u)}(x)\chi_{B(u)}(y)\,\mathrm{d}u \tag{5.19}$$

and

$$\chi*\chi((x-y)/(d\ell)) = \int\chi_{\widetilde{B}(u')}(x)\chi_{\widetilde{B}(u')}(y)\,\mathrm{d}u'. \tag{5.20}$$

It follows that

$$\int\omega_{B(u,u')}(x,y)\,\mathrm{d}u' = \omega_{B(u)}(x,y), \qquad \int\omega_{B(u)}(x,y)\,\mathrm{d}u = v_R(x-y). \tag{5.21}$$

The particle-particle interaction on the thermodynamic box Λ can therefore be found using the particle-particle interaction on the large boxes $B(u)$ and then sliding these over the thermodynamic box, i.e., by integrating with respect to u. Note that the box $B(u)$ intersects Λ if $u\ell \in \Lambda + [-\frac{\ell}{2}, \frac{\ell}{2}]^3 := \Lambda'$, and that $B(u)$ intersects Λ' if $u\ell \in \Lambda + [-\ell, \ell]^3 := \Lambda''$. With this notation we have for all $x_1, \dots, x_N \in \Lambda$

$$\begin{aligned}
&-\sum_{j=1}^{N} \rho \int v_R(x_j - y)\,\mathrm{d}y + \sum_{1\le i<j\le N} v_R(x_i - x_j) \\
&= \int\limits_{\ell^{-1}\Lambda'} \left(-\sum_{j=1}^{N} \rho \int \omega_{B(u)}(x_j, y)\,\mathrm{d}y + \sum_{1\le i<j\le N} \omega_{B(u)}(x_i, x_j) \right) \mathrm{d}u. \qquad (5.22)
\end{aligned}$$

Since we are going to work on the localization boxes, we want a simple expression for the background-background interaction on $B(u)$. Because

$$\begin{aligned}
\frac{1}{2}\rho^2 |\Lambda''| \int_{\mathbb{R}^3} v_R(x)\,\mathrm{d}x &= \int_{\mathbb{R}^3} \frac{1}{2}\rho^2 \iint\limits_{\mathbb{R}^3\times\Lambda''} \omega_{B(u)}(x, y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}u \\
&\ge \int\limits_{\ell^{-1}\Lambda'} \frac{1}{2}\rho^2 \iint \omega_{B(u)}(x, y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}u \qquad (5.23)
\end{aligned}$$

and $|\Lambda| = |\Lambda''|$ in the thermodynamic limit, we loose no precision when choosing

$$\sum_{j=1}^{N} -\rho \int \omega_{B(u)}(x, y)\,\mathrm{d}x + \sum_{1\le i<j\le N} \omega_{B(u)}(x_i, x_j) + \frac{1}{2}\rho^2 \iint \omega_{B(u)}(x, y)\,\mathrm{d}x\,\mathrm{d}y \qquad (5.24)$$

as the potential energy for the localized Hamiltonian H_B on the box $B(u)$. On the small box $B(u, u')$ we simply use

$$-\sum_{j=1}^{N} \rho \int \omega_{B(u,u')}(x_j, y)\,\mathrm{d}y + \sum_{1\le i<j\le N} \omega_{B(u,u')}(x_i, x_j) + \frac{1}{2}\rho^2 \iint \omega_{B(u,u')}(x, y)\,\mathrm{d}x\,\mathrm{d}y \qquad (5.25)$$

as the potential energy, which, after integration w.r.t. u', exactly gives (5.24). For the above arguments we could have used a smooth localization function instead.

Localization of the kinetic energy: To discuss the localization of the kinetic energy, we first introduce the projections:

- P_B denotes the orthogonal projection onto the characteristic function on B.
- Q_B is defined as $\mathbb{1}_B - P_B$.

On the N-particle sector we denote the corresponding projections onto the i^{th} particle by P_i and Q_i, defined by (2.30), and use these to define the number operators

$$n = \sum_{i=1}^{N} \mathbb{1}_{B,i}, \quad n_0 = \sum_{i=1}^{N} P_{B,i}, \quad n_+ = \sum_{i=1}^{N} Q_{B,i}.$$

The localization of the kinetic energy is quite technical but can be understood as a series of generalizations of the IMS[9] formula. We use the convention

$$\widehat{f}(p) = \int_{\mathbb{R}^3} e^{-ipx} f(x)\,\mathrm{d}x$$

[9]See [8] for a proof and historical remarks.

for the Fourier transform. With $\ell = 1$ the standard IMS formula can be written as

$$(2\pi)^{-3} p^2 * |\widehat{\chi}_u|^2 = p^2 + \int |\nabla \chi_u|^2, \tag{5.26}$$

where $\int |\nabla \chi_u|^2$ is the localization error. The first modification is to replace p^2 by a suitable function satisfying $K(p) \leq p^2$ and $K(p) = 0$ around zero. After quite some work we arrive at the following candidate for a replacement of the kinetic energy on the box $B(u)$

$$\mathcal{T}_u = Q_u \left\{ \chi_u \left[\sqrt{-\Delta} - \tfrac{1}{2}(s\ell)^{-1} \right]_+^2 \chi_u + C\ell^{-2} \right\} Q_u. \tag{5.27}$$

Here $[\,\cdot\,]_+$ denotes the positive part and $\left[\sqrt{-\Delta} - \frac{1}{2}(s\ell)^{-1} \right]_+^2$ is to be understood as multiplying by $\left[p - \frac{1}{2}(s\ell)^{-1} \right]_+^2$ in Fourier space. Since momenta of order $(\rho a)^{\frac{1}{2}}$ contribute to the ground state energy, we choose $s\ell \gg (\rho a)^{-\frac{1}{2}}$. The operator $\mathcal{T}_u$ is a good candidate, since it vanishes on constant functions, contains the gap term $C\ell^{-2} Q_u$ and satisfies

$$\int_{\mathbb{R}^3} \mathcal{T}_u \, \mathrm{d}u \leq \, -\Delta. \tag{5.28}$$

The importance of the gap term is that, provided we have a lower bound on the Hamiltonian, it will allow us to bound the amount of excited particles in states with low energy. We also want a localized kinetic energy - again including a gap term - on the small boxes $B(u, u')$ satisfying

$$\int_{\mathbb{R}^3} \mathcal{T}_{uu'} \, \mathrm{d}u' \leq \mathcal{T}_u, \tag{5.29}$$

but this seems not possible to achieve if we choose $\mathcal{T}_u$. Instead we use a modification of the operator $\mathcal{T}_u$. We define

$$\begin{aligned} \widehat{\mathcal{T}}_u = {} & \varepsilon_T (d\ell)^{-2} \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + (d\ell)^{-2}} + C\ell^{-2} Q_u \\ & + Q_u \chi_u \left\{ (1 - \varepsilon_T) \left[\sqrt{-\Delta} - \tfrac{1}{2}(s\ell)^{-1} \right]_+^2 + \varepsilon_T \left[\sqrt{-\Delta} - \tfrac{1}{2}(ds\ell)^{-1} \right]_+^2 \right\} \chi_u Q_u, \end{aligned} \tag{5.30}$$

where $0 < \epsilon_T < 1$ is a parameter and $\Delta_u^{\mathcal{N}}$ is the Neumann Laplacian on the box $B(u)$. The kinetic energy part in $\widehat{\mathcal{T}}_u$, i.e., the second line in (5.30), is slightly larger than its counterpart in (5.28) because we choose $ds\ell \ll (\rho a)^{-\frac{1}{2}}$. The important difference is the presence of the first term in (5.30), which is used to absorb error term arising from the integration over the gap term on the smaller box. When showing that

$$\int_{\mathbb{R}^3} \mathcal{T}_{uu'} \, \mathrm{d}u' \leq \widehat{\mathcal{T}}_u - C\ell^{-2} Q_u, \tag{5.31}$$

where

$$\mathcal{T}_{uu'} := C\varepsilon_T (d\ell)^{-2} Q_{uu'} + Q_{uu'} \chi_{uu'} \left[\sqrt{-\Delta} - (ds\ell)^{-1} \right]_+^2 \chi_{uu'} Q_{uu'} \tag{5.32}$$

we still have the parameter ϵ_T, which we can optimize over at the end. To save some kinetic energy, we use

$$\mathcal{T}_B := \begin{cases} (1 - \varepsilon_0) \widehat{\mathcal{T}}_u, & \text{if } B = B(u) \\ (1 - \varepsilon_0) \mathcal{T}_{uu'}, & \text{if } B = B(u, u') \end{cases} \tag{5.33}$$

and

$$H_B := \begin{cases} H_u, & \text{if } B = B(u) \\ H_{uu'}, & \text{if } B = B(u,u'). \end{cases} \tag{5.34}$$

With this notation we write the localized background Hamiltonians as

$$H_B = \sum_{i=1}^{N} \left(\mathcal{T}_{B,i} - \rho \int \omega_B(x_i, y)\,\mathrm{d}y \right) + \sum_{1\le i<j\le N} \omega_B(x_i, x_j) + \frac{1}{2}\rho^2 \iint \omega_B(x,y)\,\mathrm{d}x\,\mathrm{d}y. \tag{5.35}$$

The final result of the localization procedure are the inequalities

$$H_{\rho,N} \ge \int_{\ell^{-1}\Lambda'} \Big(-\varepsilon_0 \Delta_u^{\mathcal{N}} + H_u \Big)\,\mathrm{d}u \tag{5.36}$$

and

$$H_u - C\ell^{-2} Q_u \ge \int_{\mathbb{R}^3} H_{uu'}\,\mathrm{d}u'. \tag{5.37}$$

5.2. Expanding the Background Hamiltonian

Using $\mathbb{1}_B = P_B + Q_B$, we can write

$$-\sum_{i=1}^{N} \rho \int \omega_B(x_i, y)\,\mathrm{d}y = -\sum_{i=1}^{N} (P_{B,i} + Q_{B,i}) \rho \int \omega_B(x_i, y)\,\mathrm{d}y (P_{B,i} + Q_{B,i}) \tag{5.38}$$

and expand the particle-background interaction into 4 terms. Similarly we expand $\sum_{i<j} \omega_B(x_i, x_j)$. We organize terms by the amount of $\mathcal{Q}$-terms they contain. We define

$$\mathcal{U}_B = \frac{1}{2}|B|^{-2} \iint \omega_B(x,y)\,\mathrm{d}x\,\mathrm{d}y \tag{5.39}$$

because the background-background interaction appears frequently in our estimates. We quote the following inequality from Part II

$$\max_x \int w_B(x,y)\,\mathrm{d}y \le \frac{1}{2}C|B|^{-1} \iint w_B(x,y)\,\mathrm{d}y\,\mathrm{d}x = C|B|\mathcal{U}_B, \tag{5.40}$$

which we use for the estimates on $\mathcal{Q}_1'$.

Here we will list the different $\mathcal{Q}$-terms and give bounds in terms of n, n_0 and n_+. The background-background interaction is included into the terms with no Q:

$$\begin{aligned} \mathcal{Q}_0 :=& -\sum_i \rho P_i \int \omega_B(x_i, y)\,\mathrm{d}y P_i + \sum_{i<j} P_i P_j \omega_B(x_i, x_j) P_i P_j + \frac{1}{2}\rho^2 \iint \omega_B(x,y)\,\mathrm{d}x\,\mathrm{d}y \\ =& \left[(n_0 - \rho|B|)^2 - n_0 \right] \mathcal{U}_B = \left[|n - \rho|B||^2 - 2(n - \rho|B|)n_+ + n_+^2 - n_0 \right] \mathcal{U}_B. \end{aligned} \tag{5.41}$$

We split the terms with only one Q into two groups

$$\mathcal{Q}_1' := (n - \rho|B|)|B|^{-1} \left(\sum_i P_i \int \omega_B(x_i, y)\,\mathrm{d}y Q_i + \sum_i Q_i \int \omega_B(x_i, y)\,\mathrm{d}y P_i \right) \tag{5.42}$$

and

$$\mathcal{Q}_1'' := -|B|^{-1}\sum_i P_i \int \omega_B(x_i,y)\,\mathrm{d}y Q_i n_+ - |B|^{-1}\sum_i n_+ Q_i \int \omega_B(x_i,y)\,\mathrm{d}y P_i, \quad (5.43)$$

such that

$$\mathcal{Q}_1 = \mathcal{Q}_1' + \mathcal{Q}_1''. \quad (5.44)$$

We treat the term $\mathcal{Q}_1''$ as an error term on both the small and the large boxes. The term $\mathcal{Q}_1'$, on the other hand, we initially treat as an error term on the small boxes; thereafter we include it into the quadratic part of the Background Hamiltonian on the large boxes. We quote the following lemma.

5.2. LEMMA (Estimates on $\mathcal{Q}_1$)**.** *For all* $\varepsilon_1', \varepsilon_1''> 0$

$$\mathcal{Q}_1' \geq -\,|n-\rho|B||(\varepsilon_1' n_0 + \varepsilon_1'^{-1} C n_+)\mathcal{U}_B$$

and

$$\mathcal{Q}_1'' \geq -\,(\varepsilon_1''(n_+ + 1)n_0 + C\varepsilon_1''^{-1} n_+^2)\mathcal{U}_B.$$

Proof. Assume that A, B, C are bounded operators with B positive and A, C self-adjoint. Then

$$\langle\psi, (ABC + CBA)\psi\rangle \leq \epsilon\langle\psi, ABA\psi\rangle + \epsilon^{-1}\langle\psi, CBC\psi\rangle, \quad (5.45)$$

where we have first used the Schwarz inequality and then that $ab \leq \frac{\epsilon a^2 + \epsilon^{-1} b^2}{2}$. Using (5.40), we obtain

$$\begin{aligned}
||\mathcal{Q}_1'|| &\leq |n-\rho|B|||B|^{-1}\left[\varepsilon_1'\sum_i P_i \int \omega_B(x_i,y)\,\mathrm{d}y P_i + \varepsilon_1'^{\,-1}\sum_i Q_i \int \omega_B(x_i,y)\,\mathrm{d}y Q_i\right] \\
&\leq |n-\rho|B|||B|^{-1} n_0 \left[\varepsilon_1' \int \omega_B(x,y)\,\mathrm{d}x\,\mathrm{d}y P_i + \varepsilon_1'^{\,-1} n_+ \int \max_x \omega_B(x,y)\,\mathrm{d}y\right] \\
&\leq |n-\rho|B||\left[C\varepsilon_1' n_0 \mathcal{U}_B + C\varepsilon_1'^{\,-1} n_+ \mathcal{U}_B\right]. \quad (5.46)
\end{aligned}$$

The constant in front of ε_1' in (5.46) may be dropped by choosing ε_1' appropriately. Note also that we could have stated the lemma as a two-sided bound. The proof for the estimate on $\mathcal{Q}_1''$ is similar and can be found in Part II. □

The bound on the 3-$\mathcal{Q}$ terms is similar to the bound on $\mathcal{Q}_1''$. We have

$$\begin{aligned}
\mathcal{Q}_3 :=& \sum_{i,j} P_j Q_i \omega_B(x_i,x_j) Q_i Q_j + Q_j Q_i \omega_B(x_i,x_j) Q_i P_j \\
\geq& -\sum_{i\neq j}\left(2\varepsilon_3^{-1} P_j Q_i \omega_B(x_i,x_j) Q_i P_j + \frac{\varepsilon_3}{2} Q_j Q_i \omega_B(x_i,x_j) Q_i Q_j\right) \\
\geq& -C\varepsilon_3^{-1} n_0 n_+ \mathcal{U}_B - \varepsilon_3 \sum_{i<j} Q_j Q_i \omega_B(x_i,x_j) Q_i Q_j \\
\geq& -C\varepsilon_3^{-1} n n_+ \mathcal{U}_B - \varepsilon_3 \sum_{i<j} Q_j Q_i \omega_B(x_i,x_j) Q_i Q_j. \quad (5.47)
\end{aligned}$$

Here we used $n_0 \leq n$ for simplicity because we always have $n_0 = n$ to leading order when applying the bound on $\mathcal{Q}_3$. The last term is

$$\mathcal{Q}_4 := \sum_{i<j} Q_j Q_i \omega_B(x_i, x_j) Q_i Q_j \geq 0. \tag{5.48}$$

Without estimates on n, n_+ and $|n - \rho|B||$ we obtain no better lower bound on H_B than by using the localized Hamiltonian directly. Since all terms in (5.35) other than $\sum_i - \rho \int \omega_B(x_i, y)\, \mathrm{d}y$ are positive, we have

$$H_B \geq -Cn\rho|B|\mathcal{U}_B \geq -Cn\rho a \max \chi_B^2, \tag{5.49}$$

where (5.49) is to be understood in the sense of quadratic forms. From this a priori estimate and the gap term in the localized kinetic energy $\mathcal{T}_B$ on the small box, see (5.32), we obtain a bound on n_+.

5.3. LEMMA. *Assume that $B = B(u, u')$ and that a state Ψ satisfies $\langle H_B \rangle_\Psi := \langle \Psi, H_B \Psi \rangle \leq \frac{1}{2}\rho^2 \iint \omega_B(x, y)\, \mathrm{d}x\, \mathrm{d}y$. Then*

$$\langle n_+ \rangle_\Psi \leq C\varepsilon_T^{-1} \rho a (d\ell)^2 \langle n \rangle_\Psi \max \chi_B^2. \tag{5.50}$$

Proof. From the observation that lead to (5.49) and the gap term $C\varepsilon_T (d\ell)^{-2} Q_{uu'}$ we obtain

$$0 \geq C\varepsilon_T (d\ell)^{-2} \langle n_+ \rangle_\Psi - C\rho a \langle n \rangle_\Psi \max \chi_B^2. \tag{5.51}$$

□

Notation: We often write n_+ instead of $\langle n_+ \rangle_\Psi$.

The bounds on n and n_+ in (5.53), (5.54) and (5.55) are only valid for states with sufficiently low energy. This is no problem, since we are only interested in a lower bound for the ground state energy.

Recall that we also on the large box have a gap term, $C\ell^{-2} Q_u$. We could repeat the argument above for the large box, but since $\ell^{-2} \ll \rho a$ the result would be useless. To make the argument work on the large box, we would need an improved lower bound on the energy on the big box. Such a bound is obtained by estimating the energy on the small boxes and using (5.37). The corresponding estimate is given in Lemma 5.5.

The quadratic part: We now define the quadratic Hamiltonian, which we will treat in a similar way as described in Section 3. We define

$$H_{\mathrm{Quad}} = \sum_{i=1}^{N} (1 - \varepsilon_0) \mathcal{K}_i + \mathcal{Q}_2', \tag{5.52}$$

where $\mathcal{K}$ is the second line in (5.30) if $B = B(u)$, respectively the second term in (5.32) if $B = B(u, u')$, which are the terms that we think of as modelling the kinetic energy.

We estimate H_{Quad} using Theorem 3.1. With increasing control on n and n_+, we obtain obtain a lower bound on H_{Quad} which matches the leading order term in (5.12). At the very end we use a generalization of Theorem 3.1, which includes linear terms in $b_\pm^\sharp$ and not requires $\mathcal{B}$ to be positive. We then include $\mathcal{Q}_1'$ into the treatment of the quadratic Hamiltonian. Similar to (3.24) we add and subtract a term corresponding to the second Born term and obtain a lower bound for H_{Quad}, which is consistent with (3.28). It then remains to show that the remaining $\mathcal{Q}$-terms are of lower order.

We will now discuss how to control n and n_+ on the different boxes and how to estimate the $\mathcal{Q}$-terms which are not part of H_{Quad}.

Step 1: On small boxes for which the overlap with the large box is sufficiently large we can use the estimate on n_+ to obtain two subsequent estimates on n for states where the localized Hamiltonian has negative energy. The proof of the a priori estimate utilizes that we can split our n particles into m groups, which up to a constant factor have the same size. Because the interaction is positive, we only lower the energy if we drop the interaction between particles in different groups. If the groups have a low effective density, we can estimate the quadratic part of H_B following the approach which we outlined in Section 3 and estimate the remaining terms. For high effective densities the conditions in Lemma 3.1 can not be met, but in this case we can instead estimate H_B term by term. We arrive at the estimate

$$n \leq C|B| \max \left\{ \prod_{j=1}^{3} (\min\{\lambda_j, R\})^{-1}, \rho \right\}, \tag{5.53}$$

where λ_j is the j^{th} side length of the box $B(u, u')$.

It is unfortunate that (5.53) depends on the scaling parameter R as well as the geometry of the box since λ_j^{-1} can be arbitrarily large and we want to allow $R \ll \rho^{-\frac{1}{3}}$.

Step 2: The second step is to note that small boxes on the boundary of the large box which 'barely overlap' contribute with an energy, which is negligible. This is based on the fact that $\max \chi_B^2$ becomes very small on such boxes. We take 'barely overlap' to mean having smallest side length smaller than $\rho^{-\frac{1}{3}}$ and for such boxes the a priori bound (5.53) reduces to

$$n \leq C|B| \max \left\{ R^{-3}, \rho \right\}. \tag{5.54}$$

On these boxes we refine our a priori estimate and obtain

$$n \leq C\rho|B| \tag{5.55}$$

independently of the scaling parameter.

Step 3: With (5.55) we can bound the energy on the small box. We use $\mathcal{U}_B \leq C\frac{a}{|B|}$ to obtain

$$|n - \rho|B||n_+ \mathcal{U}_B \leq C\rho a n_+ \tag{5.56}$$

and

$$n n_+ \mathcal{U}_B \leq C\rho a n_+. \tag{5.57}$$

Our bound on n_+ does not suffice to estimate the energy of such terms directly. But if we require that $\varepsilon_T \geq C(d\ell)^2\rho a$, then we can absorb terms of size $C\rho a n_+$ into the gap term in (5.32). From the estimates on the small box we obtain by sliding the following estimate on the large box.

On the small box we started our analysis with the bound on n_+ provided by Lemma 5.3, which can not be used on the large box. Lemma 5.4 is the solution to this problem.

5.4. LEMMA. *On a large box, $B = B(u)$, we have*

$$H_B \geq 4\pi\rho^2 a_2|B| + C\ell^{-2}n_+ - C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{E}, \tag{5.58}$$

where $\mathcal{E} = \mathcal{E}(\rho, R, s, d, \ell) \gg 1$.

The term $\mathcal{E}$ is used to collect all error terms we encountered in the estimates on the small box leading to Lemma 5.4. That $\mathcal{E} \gg 1$ is what we expected from the argument on page 12 because on the small box we localized to a length scale, which is smaller than $\frac{1}{\sqrt{\rho a}}$.

5.5. LEMMA. *For any state on the large box, which satisfies*

$$\langle \psi, H_B \psi \rangle \leq 4\pi \rho^2 a_2 |B| + C\rho^2 a |B| \sqrt{\rho a^3} \mathcal{S}, \tag{5.59}$$

we have

$$n_+ \leq C\rho |B| \sqrt{\rho a^3} \mathcal{S} \tag{5.60}$$

and

$$|n - \rho|B||^2 \leq C\rho |B| \sqrt{\rho a^3} \mathcal{S}, \tag{5.61}$$

where $\mathcal{S} = \rho a \ell^2 \mathcal{E}$.

The bound on n_+ is an immediate consequence of Lemma 5.4. The estimates in Lemma 5.5 will not be improved any further.

5.3. Estimates for the error terms on the large box

With the bounds in Lemma 5.5 we can revisit the bounds on the $\mathcal{Q}$-terms. The following terms are easy to deal with:

$\mathcal{Q}_0$: The negative terms are of lower order.
$\mathcal{Q}_2'$: This term is estimated as part of the quadratic Hamiltonian.
$\mathcal{Q}_4$: This term is positive.

The remaining $\mathcal{Q}$-terms can not be estimated using Lemma 5.5. Part of the problem is that we have no good bound on n_+^2. Given a n-particle wave function Ψ, we can write Ψ as a sum of n_+ eigenfunctions, i.e.,

$$\Psi = \sum_{m=0}^{n} c_m \Psi_m, \tag{5.62}$$

where $n_+ \Psi_m = m \Psi_m$ and $||\Psi_m||_2 = 1$ for $m \in \{0, 1, \ldots, n\}$. Note that the expectation value $\langle n_+^2 \rangle_\Psi$ can be of order $\langle n \rangle_\Psi \langle n_+ \rangle_\Psi$, which is much larger than $\langle n_+ \rangle_\Psi^2$. Because we consider interaction between at most two particles, it follows that

$$\langle \Psi_m, H_B \Psi_{m'} \rangle = 0, \qquad \text{if} \quad |m - m'| \geq 3. \tag{5.63}$$

Our approach is to find a new state $\widetilde{\psi}$, which is n_+-localized and has an energy that is insignificantly higher than for the ground state. This method, which we explain below, has been introduced in [27] and also been used in [17].

n_+-localization: We quote the following theorem.

5.6. THEOREM (Localization of large matrices, (Thm. A.1, [27]))**.**
Suppose that $\mathcal{A}$ is an $(N+1)\times(N+1)$ Hermitean matrix and let $\mathcal{A}^k$, with $k = 0, 1, \ldots, N$, denote the matrix consisting of the k^{th} supra- and infra-diagonal of $\mathcal{A}$. Let $\psi \in \mathbb{C}^{N+1}$ be a normalized vector and set $d_k = \langle \psi, \mathcal{A}^k \psi \rangle$ and $\lambda = \langle \psi, \mathcal{A}\psi \rangle = \sum_{k=0}^{N} d_k$ (ψ need not be an eigenvector of $\mathcal{A}$). Choose some positive integer $\mathcal{M} \leq N + 1$. Then, with $\mathcal{M}$ fixed, there

is some $n \in [0, N+1-\mathcal{M}]$ *and some normalized vector* $\phi \in \mathbb{C}^{N+1}$ *with the property that* $\phi_j = 0$ *unless* $n+1 \leq j \leq n+\mathcal{M}$ *(i.e.,* ϕ *has length* $\mathcal{M}$*) and such that*

$$\langle \phi, \mathcal{A}\phi \rangle \leq \lambda + \frac{C}{\mathcal{M}^2} \sum_{k=1}^{\mathcal{M}-1} k^2 |d_k| + C \sum_{k=\mathcal{M}}^{N} |d_k|, \tag{5.64}$$

where $C > 0$ *is a universal constant. (Note that the first sum starts at* $k = 1$*.)*

First we translate the theorem to our setup. We use the decomposition (5.62) to define the matrix $\mathcal{A}$ via its matrix elements

$$\mathcal{A}_{m,m'} := \langle \Psi_m, H_B \Psi_{m'} \rangle \tag{5.65}$$

and define

$$\psi := (c_0, c_1, \ldots, c_n). \tag{5.66}$$

Hence

$$\langle \Psi, H_B \Psi \rangle = \langle \psi, \mathcal{A}\psi \rangle. \tag{5.67}$$

It follows from (5.63) that $d_k = 0$ for $k \geq 3$ and therefore that the second sum in (5.64) vanishes in our application. We define our n_+-localized state $\widetilde{\psi}$, using the vector ϕ in Theorem 5.6, by setting

$$\widetilde{\psi} = \sum_{m=0}^{n} \phi_m \Psi_m. \tag{5.68}$$

A simple rearrangement now gives

$$\langle \Psi, H_B \Psi \rangle \geq \langle \widetilde{\psi}, H_B \widetilde{\psi} \rangle - C\mathcal{M}^{-2} \left(|d_1| + |d_2| \right). \tag{5.69}$$

Note that we only used that our Hamiltonian satisfies (5.63) to arrive at (5.69). We choose $\mathcal{M}$ such that the last term in (5.69) is small compared to the LHY-order[10]. Then we concentrate on finding a lower bound for $\langle \widetilde{\psi}, H_B \widetilde{\psi} \rangle$. We may assume that Ψ satisfies the assumption (5.59) in Lemma 5.5. It follows that our estimates on n_+ and $|n - \rho|B||$ also apply to $\widetilde{\psi}$ and therefore that $\langle n_+ \rangle_{\widetilde{\psi}}$ is contained in the interval of possible n_+ eigenvalues of $\widetilde{\psi}$, whose length is at most $\mathcal{M}$. If we further assume that $\langle n_+ \rangle_{\widetilde{\psi}} \ll \mathcal{M}$, it follows that

$$\langle n_+^2 \rangle_{\widetilde{\psi}} \leq C \langle n_+ \rangle_{\widetilde{\psi}} \mathcal{M}. \tag{5.70}$$

Because we only use this bound to control error terms, there is no need to optimize the constant in (5.70). We identify d_1, d_2 as

$$d_1 = \langle \Psi, \left(\mathcal{Q}_1' + \mathcal{Q}_1'' + \mathcal{Q}_3 \right) \Psi \rangle \tag{5.71}$$

and

$$d_2 = \langle \Psi, \left[\sum_{i=0}^{n} Q_i Q_j \omega_B(x_i, x_j) P_i P_j + P_i P_j \omega_B(x_i, x_j) Q_i Q_j \right] \Psi \rangle. \tag{5.72}$$

We refer to Part II for the estimates showing that

$$|d_1| + |d_2| \leq C\rho^2 a |B| \frac{a}{R} = C\rho^2 a_2 |B|. \tag{5.73}$$

[10] In Part II we can not simply drop the last term in (5.69) since we also want an explicit estimate on the error terms.

We can now choose $\mathcal{M}$ such that

$$\mathcal{M}^{-2}\left(|d_1|+|d_2|\right)|B|^{-1}=o\left(\rho^2 a\sqrt{\rho a^3}\right). \tag{5.74}$$

With $-\varepsilon_0\Delta_u^{\mathcal{N}}$ being the kinetic energy which appears in (5.36), we will now show that

$$\langle\widetilde{\psi}|-\varepsilon_0\Delta_u^{\mathcal{N}}+H_B|\widetilde{\psi}\rangle|B|^{-1}\geq 4\pi\rho^2\left(a_2+\frac{128}{15\sqrt{\pi}}a((\rho a^3)^{1/2}+o((\rho a^3)^{1/2})\right). \tag{5.75}$$

Using (5.37), we lift the result from the large box to the thermodynamic box, where we obtain (5.12). Our Main Theorem 5.8 then follows from (5.11).

It remains to argue why the following terms are small compared to the LHY-order.
$\mathcal{Q}_1''$: Having n_+ being localized, we can bound the expectation in $\mathcal{Q}_1''$

$$\begin{aligned}\langle\widetilde{\psi},\mathcal{Q}_1''\widetilde{\psi}\rangle &\geq -\left(\varepsilon_1''n+C\varepsilon_1''^{-1}\mathcal{M}\right)n_+\mathcal{U}_B+\text{lower order}\\ &\geq -C\left(\rho|B|\mathcal{M}\right)^{\frac{1}{2}}\rho|B|(\rho a^3)^{\frac{1}{2}}\mathcal{S}\,\mathcal{U}_B+\text{lower order}\\ &=\text{lower order},\end{aligned} \tag{5.76}$$

provided $\mathcal{M}$ is sufficiently small.

$\mathcal{Q}_1'$: We do not estimate $\mathcal{Q}_1'$ directly. Instead we use Bogolubov's method and estimate $\mathcal{Q}_1'$ together with the quadratic part as described on page 29.

The last of the remaining $\mathcal{Q}$-terms has to be estimated in a different way than on the small box.

$\mathcal{Q}_3$: To bound the first term in (5.47), we have to choose $\varepsilon_3\gg 1$. But then we can not absorb $-\varepsilon_3\sum_{i<j}Q_jQ_i\omega_B(x_i,x_j)Q_iQ_j$ into the positive $\mathcal{Q}_4$-term as we did on the small box. Instead we use the Neumann energy $-\varepsilon_0\Delta_u^{\mathcal{N}}$, which we have saved for exactly this purpose.

A few remarks on the lower bound η for that scaling range of R are in order. For $\frac{a}{R}$ we obtain an error term which is $O(1)$ relative to the LHY-order. We make the ansatz for $\frac{R}{a}=(\rho a^3)^{-\frac{1}{3}+\eta}$ that $d=s=1$ and that $\ell=(\rho a)^{-\frac{1}{2}}$ and optimize over $\varepsilon_0,\varepsilon_T$. We arrive at the choice $\mathcal{M}=(\rho a^3)^{-\frac{1}{10}}$ and then it follow from (5.74) that $\frac{R}{a}=(\rho a^3)^{-\frac{3}{10}}$ and hence that $\eta=\frac{1}{30}$.

This concludes the description for our proof of the lower bound in Part II.

5.4. Future Work

The main drawback in our approach to the LHY-formula is that our proof for the lower bound relies on the presence of the scaling parameter R, which had to satisfy

$$(\rho a^3)^{-\nu} \ll \frac{R}{a} \ll (\rho a^3)^{-\frac{1}{2}} \tag{5.77}$$

with $\nu = \frac{3}{10}$. In future work this scaling range could be improved. Going beyond $(\rho a^3)^{-\frac{1}{4}}$ would be interesting, since it would show that the Bogolubov approximation indeed gives the correct answer.

The next big step, before completely avoiding the scaling parameter, would be only to require $\frac{R}{a} \gg (\rho a^3)^{-\epsilon}$ for any $\epsilon > 0$ or even just $R \gg a$.

If the scaling parameter could be avoided at some point, it would certainly be interesting to know not only sufficient, but also necessary conditions for the interaction potential. An intermediate step would be to show a weaker lower bound, which only covers the LHY-order, but not the right constant, i.e., showing that

$$e(\rho) \geq 4\pi\rho^2 a \left(1 + C\sqrt{\rho a^3} + o(\sqrt{\rho a^3})\right), \qquad \text{as} \quad \rho a^3 \to 0 \tag{5.78}$$

for some $C \leq \frac{128}{15\sqrt{\pi}}$.

A few necessary changes in the present approach are foreseeable already now. When we introduced the background Hamiltonian, we used for simplicity the same density for the background as for the gas. If we extend our scaling range, we should also optimize over the background density.

Another idea is to expand the background Hamiltonian into even more terms by writing $1 = \phi - (\phi - 1)$, where ϕ is the scattering solution. This idea has been utilized in [13].

A different modification of the problem would be to study the ground state energy of the dilute Bose gas – this time in D dimensions, with $D \neq 3$.

Other directions would be to study potentials with a shallow negative part, to attack the next term in the expansion, and finally, to ask to which order the ground state energy only depends on the potential through the scattering length.

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Part II

Manuscript

The Second Order Correction to the Ground State Energy of the Dilute Bose Gas

The Second Order Correction to the Ground State Energy of the Dilute Bose Gas

Birger Brietzke* Jan Philip Solovej*

QMATH
University of Copenhagen,
Universitetsparken 5, 2100 Copenhagen, Denmark
birger@math.ku.dk solovej@math.ku.dk

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Abstract

We establish the Lee–Huang–Yang formula for the ground state energy of a dilute Bose gas for a broad class of repulsive pair-interactions in 3D as a lower bound. Our result is valid in an appropriate parameter regime and confirms that the Bogolubov approximation captures the right second order correction to the ground state energy.

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Contents

1 Introduction

Bogolubov's 1947 paper [1] laid the foundation for our present theories of the ground states of dilute Bose gases. His approximate theory was intended to explain the properties of liquid Helium, but it is expected to be most accurate in the opposite regime of a dilute gas of particles (e.g., atoms) interacting pairwise with a repulsive potential $v(x_i - x_j) \geq 0$.

The simplest question that can be asked is the correctness of the prediction for the ground state energy. This, of course, can only be exact in a certain limit – the 'weak coupling' limit. In the case of the charged Bose gas that one of the authors studied [13, 14], in which particles interact via Coulomb forces, the appropriate limit is the *high density* limit. In this setting Bogolubov's prediction, first elucidated in [5], is correct to leading order in the inverse density.

In gases with short range forces, which are the object of study here, the weak coupling limit corresponds to *low density* instead. The reader is referred to [15] for background information and more details.

Our system consists of N three-dimensional particles in a large box Λ of volume $|\Lambda| = L^3$. As usual, we are interested in the thermodynamic limit $N \to \infty$, $|\Lambda| \to \infty$ with the ratio $N/|\Lambda| \to \rho$. The Hamiltonian is

$$H_N = -\nu \sum_{j=1}^{N} \Delta_j \; + \sum_{1 \leq i < j \leq N} v(x_i - x_j), \tag{1}$$

with $\nu = \hbar^2/2m$, where m is the mass of the particles. From Sect. 2 on we will set $\nu = 1$, but we leave it in place in this introduction in order to emphasize that the scattering length of v depends on ν as well as on v. We assume that $v(x) \geq 0$ and that v is spherically symmetric, i.e., $v(x) = v(|x|)$. We could assume that v is a function of sufficiently fast decay at infinity, but in order not to overburden the paper, we assume that v is of finite range, i.e., there is an R_0 such that $v(x) = 0$ for $|x| > R_0$. The ground state energy is denoted by E_N and

$$e(\rho) = \lim_{L \to \infty,\; N/|\Lambda| \to \rho} E_N/|\Lambda| \tag{2}$$

denotes the ground state energy per unit volume.

The *scattering length* a is defined by the solution of the equation $-\nu \Delta f(x) + \frac{1}{2} v(x) f(x) = 0$ that goes to 1 as $|x| \to \infty$. Such an f must satisfy $f(x) = 1 - a/|x|$ for $|x| > R_0$. If v is simply a hard-core repulsion of radius r then $a = r$.

Bogolubov's formula for the first two terms for e in a small ρ asymptotic expansion is

$$\boxed{e(\rho) = 4\pi\nu\rho^2 a\left(1+\frac{128}{15\sqrt{\pi}}\sqrt{Y}+o(\sqrt{Y})\right),} \qquad \text{with } Y=\rho a^3. \tag{3}$$

To be more exact, the leading $4\pi\nu\rho^2 a$ term was proposed by Lenz [9]. Bogolubov derived $\frac{1}{2}\rho^2\int v(x)\,\mathrm{d}x$ for the leading term by his method but, realizing that this could not be correct, noticed that $\int v(x)\,\mathrm{d}x$ is the first Born approximation to $8\pi\nu a$. The second term, while inherent in Bogolubov's work (see [10, 15]) is credited to Lee, Huang and Yang who actually derived it [8] for the hard-core gas. Again, Bogolubov's method has $\frac{1}{2}\int v(x)\,\mathrm{d}x$ in place of $4\pi\nu a$ in this term as well. It is worth noting that the naive perturbation result, $\frac{1}{2}\int v(x)\,\mathrm{d}x$, does not depend on ν, which is absurdly incorrect. Other derivations that do not use Bogolubov's setup or the momentum space formulation exist [11], but no rigorous derivation of this second term other than [7], which we discuss below, exists so far.

The first term $4\pi\nu\rho^2 a$ was attacked rigorously by Dyson [3] for the hard-core case; he proved a variational upper bound of this precise form (up to $o(\rho^2)$), as well as a lower bound that, unfortunately, was 14 times too small. He also formulated an inequality that gives a lower bound for the expectation value of v in terms of that of a longer range, softer potential. This inequality has been used in most subsequent rigorous investigations. In particular, it was essential in the paper [16] that finally proved that $4\pi\nu\rho^2 a$ is the correct leading term in three-dimensions for any $v \geq 0$ and finite range – including the hard core case.

Our focus here is on the second term. From Bogolubov's perspective it is a correlation effect and in his derivation it presupposes Bose-Einstein condensation (BEC) in the ground state. But the fact that his method gives the correct second term in *one*-dimension [12], despite the fact that there is no BEC in one-dimension, suggests that BEC may not be completely relevant for this problem.

The second term is not merely a perturbation of the first, for it involves new physics. The mean particle spacing is $\rho^{-1/3}$, which is much greater than the size of a particle (which we may take to be a, not R). The uncertainty principle tells us that the energy per particle, which is $4\pi\nu\rho a$, defines a length $\lambda = (\rho a)^{-1/2} \gg \rho^{-1/3} \gg a$ below which a particle cannot be localized without seriously altering its energy. Thus, it is totally impossible to think of individual particles in the gas; their wave-functions overlap considerably. We can also think of λ as the wavelength of the disturbance caused by dropping a particle of size $a \ll \rho^{-1/3}$ into the 'sea' of particles. The energy of this very long (on the scale of $\rho^{-1/3}$) wave, relative to the main term $\nu\rho^2 a$, can be understood heuristically from the perturbation it causes in the scattering solution resulting in a change of the (two-particle) density, $\rho \to \rho(1+O(a/\lambda))$.

This gives rise to an energy shift $\rho^2 a \to \rho^2 a(1 + O(a/\lambda)) \sim \rho^2 a(1 + O(\sqrt{Y}))$.

Until recently it seemed impossible to go beyond the methods of [16] to derive the second term in (5) rigorously. Giuliani and Seiringer [7] have made an important step forward in this quest, however, by considering a situation in which a soft potential v gets fatter and thinner as $\rho \to 0$ in such a way that $\int v$ is kept constant. In this limit the second Born approximation to the scattering length is of order v^2, and if v is soft enough one can hope for sufficient accuracy to achieve $4\pi\nu\rho^2 a$ in place of Bogolubov's $\frac{1}{2}\rho^2 \int v(x)\,\mathrm{d}x$. With the leading term sufficiently under control one can then hope to see the $\sqrt{Y}$ term. In this approach, in which the length scale of the potential is adjustable, the potential has the form

$$v_R(r) = R^{-3} v_1(r/R) \qquad \text{with } R \to \infty \text{ as } \rho \to 0. \tag{4}$$

Here v_1 is a fixed, bounded and sufficiently smooth function with finite (dimensionless) support which we take to be the unit ball such that v_R has *range* R. In [7], $v_1(r) = a_0 e^{-r}$.

The interesting question is how R depends on ρ as $\rho \to 0$. In [7] they take it to be $R \sim \rho^{-1/3-7/46}$, which implies that each particle 'sees' infinitely many others via the interaction. That is why [7] has "high density" in the title, even though the gas is low density ($a \ll \rho^{-1/3}$), and the leading term is still $4\pi\nu\rho^2 a$. Nevertheless, this is the first time that the famous $128\sqrt{Y}/15\sqrt{\pi}$ term was seen rigorously as both a lower and an upper bound. Partly relying on the ideas in [13] they achieve a proof of (5). For the upper bound a variational trial state, following [6], was used. Upper bounds corresponding to (5) were also established in [4] respectively [18], and the latter was extended to higher dimensions in [19].

Our goal is to improve the situation concerning the lower bound a bit. While we still utilize the scaling in (4), our R will also be allowed to be *less than* $\rho^{-1/3}$, which is closer to the physical situation; a particle rarely 'sees' another one now. This will require improving the methodology of [13]. In addition we shall allow for a large class of v_1.

We use the convention

$$\widehat{f}(p) = \int_{\mathbb{R}^3} e^{-ipx} f(x)\,\mathrm{d}x$$

for the Fourier transform. Our main result is:

1.1 THEOREM. *Consider a Bose gas with Hamiltonian (1) with v replaced by v_R given in (4). Assume that $v_1 \geq 0$ with support inside the unit ball, is continuous, spherically symmetric, and satisfies $v_1(0) > 0$. Assume moreover that v_1 is sufficiently regular so that, for large enough R, the scattering length a of v_R is given correctly up to order R^{-1} by the second Born approximation. Then, after taking the thermodynamic limit, the energy $e(\rho)$ is* *bounded below by*

$$e(\rho) \geq 4\pi\nu\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{Y} + o(\sqrt{Y})\right), \qquad \text{with } Y = \rho a^3, \tag{5}$$

provided

$$\lim_{\rho\to 0} R\rho^{1/3}Y^{1/6} = 0, \qquad \lim_{\rho\to 0} R\rho^{1/3}Y^{-\eta} = \infty, \tag{6}$$

where $\eta = \frac{1}{30}$.

Our error terms will depend on the dimensionless quantity $a^{-1}\int v_1 = a^{-1}R^3\int v_R$.

Remark on the Born approximation: The 'Born approximation' or 'Born series', is a formula for a as a power series in $v/8\pi\nu$.

$$a = (8\pi\nu)^{-1}\int_{\mathbb{R}^3} v(x)\,\mathrm{d}x - \sum_{k=2}^{\infty}(-8\pi\nu)^{-k}\int_{\mathbb{R}^3}(\mathcal{L}_v)^{k-1}(v)(x)\,\mathrm{d}x =: \sum_{k=1}^{\infty}\nu^{-k}a_k\ , \tag{7}$$

where $\mathcal{L}_v$ is the operator given by $\mathcal{L}_v(g)(x) = v(x)\int_{\mathbb{R}^3}|x-y|^{-1}g(y)\,\mathrm{d}y$. If each term in the series is finite for a given v, then, upon replacing v by v_R as in (4), the k^{th} term in the sum, $\nu^{-k}a_k$, will be proportional to R^{1-k}. Thus, if the series converges for some R, it will converge for all larger R. Convergence will hold for large enough R if $v \in L^1 \cap L^\infty$, but milder conditions suffice.

With the restrictions on v_1 in Theorem 1.1 we have that the Born series for a converges and may therefore write

$$a = a_1 + a_2 + O(R^{-2}) = (8\pi)^{-1}\widehat{v_R}(0) - (4\pi)^{-1}(2\pi)^{-3}\int \frac{1}{4}\widehat{v_R}(k)^2|k|^{-2}\,\mathrm{d}k + O(R^{-2}), \tag{8}$$

where we have used that $\int \frac{|\widehat{v}_1(k)|^2}{|k|^2}\,\mathrm{d}k = 2\pi^2\int\int \frac{v_1(x)\overline{v_1(y)}}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y$. The higher order corrections to a will give contributions to e that are higher order than the term we seek, namely $\rho^2 a\sqrt{Y}$.

2 Background Potential and Chemical Potential

In order to utilize the technical advantages of second quantization, it is convenient for us to work in Fock space $\mathcal{F}$ (where N takes all values ≥ 0). On Fock space we introduce a Hamiltonian H_ρ that depends on a (density) parameter ρ. Its action on the N-particle sector of Fock space is given by

$$H_{\rho,N} = \sum_{j=1}^{N} \left(-\Delta_j - \rho \int v_R(x)\,\mathrm{d}x \right) + \sum_{1\leq i<j\leq N} v_R(x_i - x_j) + \frac{1}{2}\rho^2|\Lambda| \int v_R(x)\,\mathrm{d}x. \tag{9}$$

The parameter $\nu = 1$ from now on. The box for the particles is $\Lambda = [-L/2, L/2] \in \mathbb{R}^3$ with Dirichlet boundary conditions. The introduction of the parameter ρ is equivalent to the more common grand canonical approach of adding a term $-\mu N$ with the chemical potential being $\mu = \rho \int v_R$. The last term in (9) is simply a constant depending on ρ and we add it for convenience. It is well known [17] that this grand canonical formulation is equivalent to the canonical description (fixed N) that we started with, but we will not use this fact. In this paper we will focus on the background Hamiltonian H_ρ and its thermodynamic ground state energy per volume

$$e_0(\rho) = \lim_{|\Lambda|\to\infty} |\Lambda|^{-1} \inf_{\Psi\in\mathcal{F}, \|\Psi\|=1} \langle \Psi | H_\rho | \Psi \rangle.$$

The ground state energy of H_ρ is of course the same as the ground state energy of $H_{\rho,N}$ minimized over N. The Fock space may seem irrelevant since H_ρ conserves particle number, but we will later on introduce particle non-conserving operators in our analysis. Our main result is a lower bound on $e_0(\rho)$.

2.1 THEOREM (Ground state of background Hamiltonian)**.**
The thermodynamic ground state energy per volume of H_ρ satisfies the asymptotics

$$e_0(\rho) \geq 4\pi\rho^2 \left(a_2 + \frac{128}{15\sqrt{\pi}} a(Y^{1/2} + o(Y^{1/2})) \right) \tag{10}$$

as $\rho \to 0$ if

$$\lim_{\rho\to 0} R\rho^{1/3} Y^{1/6} = 0, \qquad \lim_{\rho\to 0} R\rho^{1/3} Y^{-\eta} = \infty \tag{11}$$

with η as in Theorem 1.1. Here a is the scattering length of v_R, a_2 is the second term in the Born series (7) for a, and $Y = \rho a^3$. If $R = \rho^{-\frac{1}{3}}(\rho a^3)^\mu$ with $\mu \in (-\frac{1}{6}, \frac{1}{30})$, then the error term in (10) *can be bounded by*

$$C\rho^2 a(\rho a^3)^{\frac{1}{2}+\omega} \tag{12}$$

with $\omega = \omega(\rho, \mu) > 0$.

We will now prove the main result Theorem 1.1 from Theorem 2.1.

Proof of Theorem 1.1. By choosing a trial state for $H_{\rho,N}$ corresponding to the ground state for H_N, we obtain in the thermodynamic limit that

$$\begin{aligned} e(\rho) &\geq e_0(\rho) + \lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} \rho \frac{N}{|\Lambda|} \int v_R - \frac{1}{2}\rho^2 \int v_R \\ &= e_0(\rho) + \frac{1}{2}\rho^2 \int v_R. \end{aligned}$$

If we recall that $\int v_R = 8\pi a_1$, we find from Theorem 2.1 that as $\rho \to 0$

$$\begin{aligned} e(\rho) &\geq 4\pi\rho^2 \left(a_2 + \frac{128}{15\sqrt{\pi}} a (Y^{1/2} + O(Y^{1/2+\omega})) \right) + 4\pi a_1 \rho^2 \\ &= 4\pi\rho^2 \left(a_1 + a_2 + \frac{128}{15\sqrt{\pi}} a (Y^{1/2} + O(Y^{1/2+\omega})) \right) \\ &= 4\pi\rho^2 a \left(1 + \frac{128}{15\sqrt{\pi}} Y^{1/2} + O(Y^{1/2+\omega}) \right), \end{aligned}$$

where we have used that $\frac{a_1+a_2}{a} = 1 + O(\frac{a^2}{R^2}) = 1 + o(Y^{2/3-2\eta}) = 1 + o(Y^{1/2+\omega})$.

□

Notation: In our setup the ratio of the scattering length a to $\int v_R$ is bounded above and below by constants. In all our error bounds there is therefore no point in distinguishing between $\int v_R$ and a. We choose to write the estimates in terms of a.
The rest of the paper will be devoted to the proof of Theorem 2.1.

3 Localization

As usual in the rigorous theory of the ground state energy of the Bose gas we find it necessary to localize the particles into boxes of a certain definite size. This achieves two goals. One is the control of the local fluctuations in particle number and the other is to create a gap in the spectrum of the kinetic operator, which allows us to assert that most particles are in the lowest state of the kinetic energy operator, i.e., they are effectively Bose-condensed on the scale of the box. Alas, this does not allow us to prove Bose-Einstein condensation in the thermodynamic limit, but for the purpose of computing the ground state energy local condensation suffices.

Because there are several length scales, it will turn out to be necessary to localize twice into boxes of two different sizes. The physical length scales of the problem that we are interested in are the following

$$a \ll R \ll \rho^{-1/3} \ll (\rho a)^{-1/2} \tag{13}$$

and these have the following interpretations:

- a is the scattering length of the two-body potential, v_R.
- R is the range of the potential in case it has compact support and in general it describes the length scale on which the potential vanishes. In our treatment R will be required to be much larger than a.
- $\rho^{-1/3}$ is the mean particle spacing.
- $(\rho a)^{-1/2}$ is the distance determined by the uncertainty principle given that the energy per particle is approximately ρa. In other words if one throws a particle into the gas it makes a splash of size $(\rho a)^{-1/2}$. In fact, $(\rho a)^{-1/2}$, sometimes called the healing length, is the typical distance between the particles in the virtual pairs in the Bogolubov Theory. Momenta of the order of $(\rho a)^{1/2}$ are responsible for the second term in (5).

The theorem that we prove includes a bigger range than indicated by (13). If we write $R = \rho^{-1/3} Y^{\mu}$ then, as stated in Theorem 1.1, μ can range in $(-\frac{1}{6}, \eta)$ with $\eta = \frac{1}{30}$.

The box sizes we are concerned with for localization are ℓ and $d\ell$, where $d \ll 1$ in such a way that $\ell \gg (\rho a)^{-1/2} \gg d\ell \gg \rho^{-1/3}$. Below we will also introduce a small parameter $s > 0$ and the length scales $s\ell$ and $ds\ell$. This will give the complete list of length scales

$$a \ll R, \rho^{-1/3} \ll ds\ell \ll d\ell \ll (\rho a)^{-1/2} \ll s\ell \ll \ell. \tag{14}$$

Although in Theorem 2.1 we also allow R to be much larger than $\rho^{-1/3}$, the physically interesting case is, of course, $R \ll \rho^{-1/3}$. To be precise, we will in the rest of the paper assume that the following conditions are satisfied.

CONDITION 1: *There is a sufficiently small constant* $0 < \delta < 1$ *(to be specified in the course of the paper) such that* $a, R, s, d, \ell, \rho > 0$ *satisfy*

$$a/R < \delta, \qquad \rho a^3 < \delta, \qquad \rho^{-\frac{1}{3}}(ds\ell)^{-1} < \delta, \qquad s < \delta,$$
$$d\ell(\rho a)^{1/2} < \delta, \qquad R(ds\ell)^{-1} < \delta, \qquad (\rho a)^{-1/2}(s\ell)^{-1} < \delta.$$

In particular $d < s\delta^2$.

More (and stronger) conditions will be added later. As explained, δ will be chosen in the course of the paper. It will depend on v_1 and on the integer M, which we introduce in (16) below. The integer M will however be chosen at the end and then δ really depends only on v_1.

For $u \in \mathbb{R}^3$ we introduce the notation $\Gamma_u = u + [-1/2, 1/2]^3$ for the unit cube centered at u. There are three kinds of boxes to be considered. The first is $B(u) = \ell\,\Gamma_u$, which is a cube of side length ℓ and center ℓu. The second kind is the smaller cube $\widetilde{B}(u') = (d\ell)\,\Gamma_{u'}$ of side length $d\ell$ and center $d\ell u'$. Finally, we have the rectangles $B(u,u') = B(u) \cap \widetilde{B}(u')$, which occur when the smaller box is only partially inside the larger box. The second kind is really just a special case of the third kind, so we will not introduce a name for it at this point. Generically, we will let B denote any of these boxes. We denote the side lengths of B by $\lambda_1 \le \lambda_2 \le \lambda_3$.

We now introduce a localization function $0 \le \chi \in C_0^M(\mathbb{R}^3)$ where M is an integer that we choose later. Let

$$\zeta(y) = \begin{cases} \cos(\pi y), & \text{if } |y| \le 1/2 \\ 0, & \text{if } |y| \ge 1/2 \end{cases} \tag{15}$$

and define

$$\chi(x) = C_M \big(\zeta(x_1)\, \zeta(x_2)\, \zeta(x_3) \big)^{M+1}. \tag{16}$$

Here C_M is chosen such that $\int \chi^2 = 1$. Under these conditions χ is indeed a C_0^M function and $\max \chi = \chi(0) = C_M > 0$.

It is important not to choose χ to be infinitely differentiable since the proof of Lemma 3.2 exploits that ζ is concave on its support. We shall eventually choose M to be some fixed integer. In the following all constants will depend on M, but we shall mostly omit this fact.

For $u \in \mathbb{R}^3$ we write $\chi_u(x) = \chi(x\ell^{-1} - u)$ for the localization function corresponding to the box $B(u)$. The localization function for the box $B(u,u')$ is $\chi_u(x)\chi_{u'}(x/d)$. We introduce the notation

$$\chi_B(x) = \begin{cases} \chi_u(x), & \text{if } B = B(u) \\ \chi_u(x)\chi_{u'}(x/d), & \text{if } B = B(u,u') \end{cases} \tag{17}$$

and note that

$$\int \chi_u^2(x)\, \mathrm{d}u = 1, \qquad \int \chi_u^2(x)\, \mathrm{d}x = \ell^3 \qquad \text{and} \qquad \int \chi_{B(u,u')}^2(x)\, \mathrm{d}u' = \chi_{B(u)}^2(x). \tag{18}$$

Note that if $B = B(u,u')$ is a small box with smallest side length $\lambda_1 < d\ell$, we have the bound

$$\max \chi_B^2 \leq C \left[\left(\frac{\lambda_1}{\ell}\right)^{M+1} \left(\frac{|B|}{(d\ell)^3}\right)^{M+1} \right]^2 \leq C \left(\frac{\lambda_1}{d\ell}\right)^{4(M+1)}, \tag{19}$$

which becomes useful in situations where λ_1 is small.

3.1 Localization of the Potential

Corresponding to the interaction potential v_R, we define two new potentials

$$W_{\mathrm{b}}(x) := \frac{v_R(x)}{(\chi * \chi)(x/\ell)} \tag{20}$$

and

$$W_{\mathrm{s}}(x) := \frac{W_b(x)}{[(\chi * \chi)(x/(d\ell))]} = \frac{v_R(x)}{[(\chi * \chi)(x/\ell)]\,[(\chi * \chi)(x/(d\ell))]}\,. \tag{21}$$

Here the subscripts b and s refer to the size of the box (big or small). We will mostly omit this subscript as long as the context is clear. Note that $W_{\mathrm{s,b}}$ is well defined, since by Condition 1 the range R of v_R is smaller than the scaled range of χ, which is at least of order $d\ell$. Thus whenever the denominator vanishes, then the numerator is already zero. Since $\chi * \chi$ is a symmetric C^{2M} function and because $(\chi * \chi)(0) = \int \chi^2 = 1$, we get the estimates

$$v_R(x) \leq W_b(x) \leq (1 + C(\tfrac{R}{\ell})^2) v_R(x), \tag{22}$$

$$v_R(x) \leq W_s(x) \leq (1 + C(\tfrac{R}{d\ell})^2) v_R(x). \tag{23}$$

We introduce localized potentials

$$w_B(x,y) := \chi_B(x) W_{\mathrm{b,s}}(x-y) \chi_B(y) = \chi_B(x) W(x-y) \chi_B(y), \tag{24}$$

where b is used if the box B is big, i.e., of the form $B(u)$ and s is used if B is small, i.e., of the form $B(u,u')$. As indicated on the right, we will often omit b and s. Recall that also the form of the localization functions depends on whether the box is big or small. The potential w_B is localized to the box B.

Because we do not want to have to consider boxes at the boundary of Λ throughout this paper, we introduce $\Lambda' := \Lambda + [-\frac{\ell}{2}, \frac{\ell}{2}]^3$ and $\Lambda'' := \Lambda + [-\ell, \ell]^3$. Note that $B(u)$ intersects Λ exactly if $u\ell \in \Lambda'$. Replacing the last term in (9) by $\frac{1}{2}\rho^2 |\Lambda''| \int v_R(x)\,\mathrm{d}x$ does not change the ground state energy of H_ρ in the thermodynamic limit. We may therefore use the following localization for the potential energy.

3.1 PROPOSITION (Potential localization). *For all $x_1,\ldots,x_N\in\Lambda$ we have*

$$
\begin{aligned}
&-\sum_{j=1}^N \rho\int v_R(x_j-y)\,\mathrm{d}y+\sum_{1\le i<j\le N} v_R(x_i-x_j)+\frac12\rho^2|\Lambda''|\int v_R(x)\,\mathrm{d}x\\
&=\int_{\mathbb{R}^3}\left(-\sum_{j=1}^N\rho\int \omega_{B(u)}(x_j,y)\,\mathrm{d}y+\sum_{1\le i<j\le N}\omega_{B(u)}(x_i,x_j)+\frac12\rho^2\iint_{\mathbb{R}^3\times\Lambda''}\omega_{B(u)}(x,y)\,\mathrm{d}x\,\mathrm{d}y\right)\,\mathrm{d}u\\
&\ge\int_{\ell^{-1}\Lambda'}\left(-\sum_{j=1}^N\rho\int \omega_{B(u)}(x_j,y)\,\mathrm{d}y+\sum_{1\le i<j\le N}\omega_{B(u)}(x_i,x_j)+\frac12\rho^2\iint \omega_{B(u)}(x,y)\,\mathrm{d}x\,\mathrm{d}y\right)\,\mathrm{d}u,
\end{aligned}
$$

where $\Lambda':=\Lambda+[-\frac{\ell}{2},\frac{\ell}{2}]^3$ and $\Lambda'':=\Lambda+[-\ell,\ell]^3$. Moreover, for all $u\in\mathbb{R}^3$,

$$
\begin{aligned}
&-\sum_{j=1}^N \rho\int \omega_{B(u)}(x_j,y)\,\mathrm{d}y+\sum_{1\le i<j\le N}\omega_{B(u)}(x_i,x_j)+\frac12\rho^2\iint \omega_{B(u)}(x,y)\,\mathrm{d}x\,\mathrm{d}y\\
&=\int_{\mathbb{R}^3}\left(-\sum_{j=1}^N\rho\int \omega_{B(u,u')}(x_j,y)\,\mathrm{d}y+\sum_{1\le i<j\le N}\omega_{B(u,u')}(x_i,x_j)+\frac12\rho^2\iint \omega_{B(u,u')}(x,y)\,\mathrm{d}x\,\mathrm{d}y\right)\,\mathrm{d}u'.
\end{aligned}
$$

Proof. This follows from the identity $(\chi*\chi)(x-y)=\int\chi(x-u)\chi(y-u)\,\mathrm{d}u$. □

The background self-energy appears so frequently that we shall denote it $\rho^2|B|^2\mathcal{U}_B$, i.e., we introduce the symbol

$$
\boxed{\mathcal{U}_B=\frac12|B|^{-2}\iint w_B(x,y)\,\mathrm{d}x\,\mathrm{d}y.} \tag{25}
$$

In a large box $B(u)$ the quantity $\mathcal{U}_B$ is bounded above and below by $C\frac{a}{|B(u)|}=C\frac{a}{\ell^3}$. In a small (possibly rectangular) box B, $\mathcal{U}_B$ may be significantly different. It will be important to know the following facts.

3.2 LEMMA. *If B is either a large or a small box (side lengths $\lambda_1\le\lambda_2\le\lambda_3$), there is a constant C that depends only on M used in the definition of χ and on the potential v_1 in (4) such that*

$$
\max_x\int w_B(x,y)\,\mathrm{d}y\le\frac12 C|B|^{-1}\iint w_B(x,y)\,\mathrm{d}y\,\mathrm{d}x=C|B|\mathcal{U}_B \tag{26}
$$

$$
C^{-1}\frac{a}{|B|R^3}\max\chi_B^2\prod_{j=1}^3\min\{\lambda_j,R\}\le\mathcal{U}_B\le C\frac{a}{R^3}\max\chi_B^2 \tag{27}
$$

$$\mathcal{U}_B \le C\frac{a}{|B|}\max \chi_B^2. \tag{28}$$

(The scattering length a, which obviously is bounded above and below by constants depending only on v_1, has been included in this inequality for dimensional reasons.)

Proof. The difficult case is a (possibly) rectangular box $B = B(u, u')$, for the large cubic boxes $B = B(u)$ the argument is the same just simpler. Recall that for a small box we have $w_B(x, y) = \chi_B(x)W_{\rm s}(x-y)\chi_B(y)$ and $\chi_B(x) = \chi_1(x_1)\chi_2(x_2)\chi_3(x_3)$, where

$$\chi_i(x_i) = C_M^{2/3}\zeta(|(x_i/\ell) - u_i|)^{M+1}\zeta(|(x_i/(d\ell)) - u_i'|)^{M+1}$$

for $i = 1, 2, 3$. The function χ_i is supported on an interval I_i of length λ_i corresponding to a side length of the box. We have $0 < \lambda_i \le d\ell$. Let I_i' denote the middle third of this interval. Since ζ is positive and concave on its support, it is a straightforward exercise to check that

$$\inf_{x_i\in I_i'} \chi_i(x_i) \ge c \max_{x_i\in I_i} \chi_i(x_i) \tag{29}$$

for $i = 1, 2, 3$, where $c> 0$ depends only on M. It is important here that χ is not infinitely differentiable.

By (4), (23) and the fact that v_1 is continuous has compact support and $v_1(0) > 0$ we may assume that there are constants $C_1, C_2 > 0$ (depending only on v_1) such that

$$C_1\prod_{i=1}^{3} \mathbb{1}_{[-C_1R,C_1R]}(x_i) \le a^{-1}R^3W_{\rm s}(x) \le C_2\prod_{i=1}^{3} \mathbb{1}_{[-C_2R,C_2R]}(x_i),$$

where $\mathbb{1}_I$ is the characteristic function of the interval I. To prove the inequality (26), it is therefore enough to prove the 1-dimensional versions:

$$\max_{x_i\in\mathbb{R}}\int \chi_i(x_i)\mathbb{1}_{[-C_2R,C_2R]}(x_i-y_i)\chi_i(y_i)\,{\rm d}y_i \le C\lambda_i^{-1}\iint \chi_i(x_i)\mathbb{1}_{[-C_1R,C_1R]}(x_i-y_i)\chi_i(y_i)\,{\rm d}y_i\,{\rm d}x_i,$$

for $i = 1, 2, 3$, where C is allowed to depend only on v_1 and M. In view of (29) this follows from

$$\max_{x_i\in\mathbb{R}}\int_{I_i} \mathbb{1}_{[-C_2R,C_2R]}(x_i - y_i)\,{\rm d}y_i \le C\lambda_i^{-1}\iint_{I_i'\times I_i'} \mathbb{1}_{[-C_1R,C_1R]}(x_i - y_i)\,{\rm d}y_i\,{\rm d}x_i.$$

This is obvious since both sides can be estimated above and below by constants times $\min\{\lambda_i, R\}$.

The lower bound in (27) is proved in a similar fashion. The upper bound in (27) follows from $v_R(x) \le C\frac{a}{R^3}$.

For the bound in (28) we note that $\mathcal{U}_B \le C|B|^{-1}\int_{\mathbb{R}^3} v_R(x)\max\chi_B^2\,{\rm d}x \le C\frac{a}{|B|}\max\chi_B^2,$

since $\omega_B(x,y) \le Cv_R(x-y)\max\chi_B^2$ and that by Condition 1 we have $\int v_R(x)\,\mathrm{d}x \le Ca$. $\square$

3.2 Localization of the Kinetic Energy

Let θ be the characteristic function of the cubic box $[-1/2,1/2]^3$. For $u \in \mathbb{R}^3$ we denote the corresponding characteristic function of the box $B(u)$ by $\theta_u(x) = \theta(x\ell^{-1} - u)$. We shall also use the localization function $\chi_u(x) = \chi(x\ell^{-1} - u)$ introduced on page 3.

We define the operator Q_u to be the orthogonal projection on $L^2(\mathbb{R}^3)$ defined by

$$Q_u f = \theta_u f - \ell^{-3}\langle\theta_u|f\rangle\theta_u. \tag{30}$$

In other words $Q_u f$ is a function in $L^2(\mathbb{R}^3)$ that is zero outside the box $B(u)$ and is orthogonal to the constant functions in the box.

3.3 LEMMA (Abstract kinetic energy localization)**.** *Let $K : \mathbb{R}^3 \to [0,\infty)$ be a symmetric, continuous function, which is bounded by a polynomial of degree of most $2M$, where M is the constant introduced in* (16)*. We use it to define an operator on $L^2(\mathbb{R}^3)$ by*

$$T = \int_{\mathbb{R}^3} Q_u\chi_u K(-i\ell\nabla)\chi_u Q_u\,\mathrm{d}u, \tag{31}$$

where χ_u is considered here as a multiplication operator in configuration space. This T is translation invariant, i.e., a multiplication operator in Fourier space $T = F(-i\ell\nabla)$, with

$$F(p) = (2\pi)^{-3}K * |\widehat{\chi}|^2(p) - 2(2\pi)^{-3}\widehat{\theta}(p)\widehat{\chi} * (K\widehat{\chi})(p) + (2\pi)^{-3}\left(\int K|\widehat{\chi}|^2\right)\widehat{\theta}(p)^2. \tag{32}$$

In particular, we have $F(0) = 0$.

Proof. By a simple scaling it is enough to consider $\ell = 1$. This is a straightforward calculation. Note that Q_u has the integral kernel $\theta_u(y)\,[\delta(y-x) - \mathbb{1}]\,\theta_u(x)$. If we denote by $\check{K}$ the inverse Fourier transform of K, then the integral kernel of the operator $Q_u\chi_u K(-i\nabla)\chi_u Q_u$ is given by

$$\begin{aligned}&\chi_u(x)\check{K}(x-y)\chi_u(y) - \chi_u(x)[\check{K} * \chi_u](x)\theta_u(y)\\ &-\theta_u(x)[\check{K} * \chi_u](y)\chi_u(y) + \theta_u(x)\langle\chi_u|K(-i\nabla)\chi_u\rangle\theta_u(y).\end{aligned}$$

Thus the integral kernel of $\int Q_u\chi_u K(-i\nabla)\chi_u Q_u\,\mathrm{d}u$ is given by

$$([\chi * \chi]\check{K})(x-y) - 2\left(\chi[\check{K} * \chi]\right) * \theta(x-y) + (2\pi)^{-3}\left(\int K(p)\widehat{\chi}(p)^2\,\mathrm{d}p\right)\theta * \theta(x-y),$$

where we used that $\int K(p)\widehat{\chi}(p)^2\,\mathrm{d}p$ is finite by the choice of K. We arrive at the expression for F by calculating the inverse Fourier transform. The fact that $F(0)=0$ follows since $\widehat{\theta}(0)=\int\theta=1$ and

$$(2\pi)^3F(0)=2\left(\int K\widehat{\chi}^2\right)(1-\widehat{\theta}(0))^2=0.$$

□

With $\ell=1$ this lemma is similar to the generalized IMS localization formula

$$\int_{\mathbb{R}^3}\chi_u K(-i\nabla)\chi_u\,\mathrm{d}u=(2\pi)^{-3}K*|\widehat{\chi}|^2,$$

where $K(p)=p^2$ gives the standard IMS formula since $(2\pi)^{-3}K*|\widehat{\chi}|^2=p^2+\int|\nabla\chi|^2$.

3.4 COROLLARY. *With the same notation as above we have that*

$$\int_{\mathbb{R}^3}Q_u\,\mathrm{d}u=1-\widehat{\theta}(-i\ell\nabla)^2, \tag{33}$$

i.e., the operator $\int_{\mathbb{R}^3}Q_u\,\mathrm{d}u$ is the multiplication operator in Fourier space given by $1-\widehat{\theta}(\ell p)^2$.

Proof. Simply take $K=1$ and $\chi=\theta$ in the above lemma. □

We will use Lemma 3.3 for the function $K(p)=((|p|-s^{-1})_+)^2$, where $s>0$ is the parameter introduced in Condition 1. Here $u_+=\max\{u,0\}$ denotes the positive part of u and we will henceforth write u_+^2 instead of $(u_+)^2$. Note that $|-i\nabla|=\sqrt{-\Delta}$.

3.5 LEMMA. *There is a constant $C>0$ (depending on the integer M in the definition (16) of χ) such that we have the operator inequality*

$$\int Q_u\chi_u\left[\sqrt{-\Delta}-(s\ell)^{-1}\right]_+^2\chi_uQ_u\,\mathrm{d}u\le F_s(\sqrt{-\Delta}), \tag{34}$$

where

$$F_s(|p|)=\begin{cases}(|p|-\frac{1}{2}(s\ell)^{-1})^2, & \text{if } |p|\ge\frac{5}{6}(s\ell)^{-1}\\ Cs^{M-2}p^2, & \text{if } |p|<\frac{5}{6}(s\ell)^{-1}\end{cases}, \tag{35}$$

(assuming $M\ge1$).

Proof. We may again by a simple scaling argument assume $\ell=1$. Since we defined χ in (16) as an C_0^M function, we have for $n\le 2M$ and C only depending on M that

$$\int_{|q|>s^{-1}}|q|^n\widehat{\chi}^2(q)\,\mathrm{d}q\le s^{2M-n}\int_{|q|>s^{-1}}|q|^{2M}\widehat{\chi}^2(q)\,\mathrm{d}q\le Cs^{2M-n}. \tag{36}$$

We use (31) and (32) with $K(p) = [|p| - s^{-1}]_+^2$. For the first term in (32) we find

$$\begin{aligned}(2\pi)^{-3} K * \widehat{\chi}^2(p) &\leq (2\pi)^{-3} \int (|p-q| - s^{-1})^2 \widehat{\chi}^2(q)\,\mathrm{d}q \\ &\leq (2\pi)^{-3} \int (p^2 - 2pq + q^2 - 2s^{-1}(|p| - |q|) + s^{-2}) \widehat{\chi}^2(q)\,\mathrm{d}q \\ &= (|p| - s^{-1})^2 + (2\pi)^{-3} \int q^2 \widehat{\chi}^2(q)\,\mathrm{d}q + 2(2\pi)^{-3} s^{-1} \int |q| \widehat{\chi}^2(q)\,\mathrm{d}q \\ &\leq (|p| - s^{-1})^2 + Cs^{-1},\end{aligned}$$

where we have used $(2\pi)^{-3} \int q^2 \widehat{\chi}(q)^2\,\mathrm{d}q = \int |\nabla\chi|^2$, that χ^2 is even and that $s < 1$ by Condition 1. If $|p| \geq \frac{5}{6}s^{-1}$ we find

$$(2\pi)^{-3} K * \widehat{\chi}^2(p) \leq (|p| - \frac{1}{2}s^{-1})^2 - \frac{1}{12}s^{-2} + Cs^{-1}.$$

For the second term in (32) we find since $\widehat{\theta} \leq 1$ that

$$|\widehat{\theta}(p) \widehat{\chi} * (K\widehat{\chi})(p)| \leq ||\widehat{\chi}||_2 ||K\widehat{\chi}||_2 \leq C \left(\int_{|q| \geq s^{-1}} |q|^4 |\widehat{\chi}(q)|^2\,\mathrm{d}q \right)^{1/2} \leq Cs^{M-2}. \tag{37}$$

For the third term in (32) we have similarly

$$|\widehat{\theta}(p)|^2 \int K |\widehat{\chi}|^2 \leq \int_{|q| \geq s^{-1}} |q|^2 \widehat{\chi}(q)^2\,\mathrm{d}q \leq Cs^{2M-2}. \tag{38}$$

Thus for $|p| \geq \frac{5}{6}s^{-1}$ and $s < 1$ we have that the function F in (32) satisfies

$$F(p) \leq (|p| - \frac{1}{2}s^{-1})^2 - \frac{1}{12}s^{-2} + Cs^{-1}.$$

Hence if by Condition 1 s is small enough, we arrive at the first line in (35).

We turn to the proof of the second line in (35). We know that $F(0) = 0$. Moreover since $F \geq 0$ we must have $\nabla F(0) = 0$. The lemma follows from Taylor's formula if we can show that for $|p| < \frac{5}{6}s^{-1}$, we have

$$|\partial_i \partial_j F(p)| \leq Cs^{M-2}. \tag{39}$$

It is straightforward to see that all second derivatives of $K(p) = [|p| - s^{-1}]_+^2$ are bounded independently of s. For the first term in (32) we thus find for $|p| < \frac{5}{6}s^{-1}$

$$|\partial_i \partial_j (K * \widehat{\chi}^2)(p)| = |(\partial_i \partial_j K) * \widehat{\chi}^2(p)| \leq C \int_{|p-q| > s^{-1}} \widehat{\chi}(q)^2\,\mathrm{d}q$$

$$\leq C \int_{|q|>(6s)^{-1}} \widehat{\chi}(q)^2 \, \mathrm{d}q \leq C s^{2M}.$$

For the second and third term in (32) we use the fact that the numbers

$$\|\widehat{\theta}\|_\infty, \ \|\partial_i \widehat{\theta}\|_\infty, \ \|\partial_i\partial_j \widehat{\theta}\|_\infty, \ \int |\widehat{\chi}|^2, \ \int |\partial_i \widehat{\chi}|^2, \ \int |\partial_i\partial_j \widehat{\chi}|^2,$$

for all $i, j = 1, 2, 3$ are all bounded above by a constant. The same estimates that led to (37) and (38) then imply (39). □

3.6 COROLLARY. *If $M \geq 3$ we obtain the operator inequality*

$$\int_{\mathbb{R}^3} Q_u \left\{ \chi_u \left[\sqrt{-\Delta} - \tfrac{1}{2}(s\ell)^{-1} \right]_+^2 \chi_u + b\ell^{-2} \right\} Q_u \, \mathrm{d}u \leq -\Delta,$$

provided b is smaller than some universal constant (that we shall not attempt to evaluate).

Proof. We again consider $\ell = 1$. Note that by Corollary 3.4 we have

$$\int Q_u \, \mathrm{d}u \leq \beta^{-1} \frac{-\Delta}{-\Delta + \beta} \tag{40}$$

for a universal constant $0 < \beta < 1$. We use the previous lemma with s replaced by $2s$. We then find that

$$\int_{\mathbb{R}^3} Q_u \chi_u \left[\sqrt{-\Delta} - \tfrac{1}{2} s^{-1} \right]_+^2 \chi_u Q_u \, \mathrm{d}u + b \int_{\mathbb{R}^3} Q_u \, \mathrm{d}u \leq F_{2s}(\sqrt{-\Delta}) + b\beta^{-1} \frac{-\Delta}{-\Delta + \beta}.$$

For $|p| < (5/12)s^{-1}$ Lemma 3.5 gives

$$F_{2s}(p) + b\beta^{-1} \frac{p^2}{p^2 + \beta} \leq C s p^2 + b\beta^{-1} \frac{p^2}{p^2 + \beta} \leq (Cs + b\beta^{-2}) p^2 \leq p^2$$

for s and b small enough. For $|p| \geq (5/12)s^{-1}$ we find from Lemma 3.5 that

$$F_{2s}(p) + b\beta^{-1} \frac{p^2}{p^2 + \beta} \leq (|p| - \frac{1}{4} s^{-1})^2 + b\beta^{-1} \frac{p^2}{p^2 + \beta} \leq p^2 - \frac{5}{24} s^{-2} + \frac{1}{16} s^{-2} + b\beta^{-1} \leq p^2,$$

for s and b small enough. □

This corollary will allow us to localize the kinetic energy to boxes. What will be left as the kinetic energy in the box $B(u)$ centered at ℓu, is the operator

$$\mathcal{T}_u = Q_u \left\{ \chi_u \left[\sqrt{-\Delta} - \tfrac{1}{2}(s\ell)^{-1} \right]_+^2 \chi_u + b\ell^{-2} \right\} Q_u. \tag{41}$$

Note that $\mathcal{T}_u$ vanishes on constant functions. The last term in $\mathcal{T}_u$ will control the gap in the kinetic energy, i.e., on functions orthogonal to constants in the box, $\mathcal{T}_u$ is bounded below by at least $b\ell^{-2}$.

As explained above, we need to localize even further to smaller boxes whose size is a factor $d \ll 1$ smaller than the larger box. In these smaller boxes we also need a term in the kinetic energy that gives a gap. Unfortunately, the above expression (41) for the kinetic energy does not immediately allow for such further localization. For this reason we must introduce a more complicated kinetic energy in the larger box.

We will use

$$\begin{aligned}\widehat{\mathcal{T}}_u &= \varepsilon_T (d\ell)^{-2} \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + (d\ell)^{-2}} + b\ell^{-2} Q_u \\ &+ Q_u \chi_u \left\{ (1-\varepsilon_T) \left[\sqrt{-\Delta} - \tfrac{1}{2}(s\ell)^{-1}\right]_+^2 + \varepsilon_T \left[\sqrt{-\Delta} - \tfrac{1}{2}(ds\ell)^{-1}\right]_+^2 \right\} \chi_u Q_u,\end{aligned} \tag{42}$$

where $0 < \varepsilon_T < 1$ is a parameter. The operator $\Delta_u^{\mathcal{N}}$ is the Neumann Laplacian on the box $B(u)$. As usual Δ is the Laplacian on $\mathbb{R}^3$. Let us be clear about the action of $\Delta_u^{\mathcal{N}}$ as an operator on $L^2(\mathbb{R}^3)$. It is the operator associated with the quadratic form

$$(f, -\Delta_u^{\mathcal{N}} f) = \int_{B(u)} |\nabla f(x)|^2 \, \mathrm{d}x,$$

which is defined for all functions $f \in L^2(\mathbb{R}^3)$ whose restriction to the cube is an H^1 function on the cube, i.e., functions for which the above integral is finite. Note that by the operator $(-\Delta_u^{\mathcal{N}} + (d\ell)^{-2})^{-1}$ we mean the inverse of $-\Delta_u^{\mathcal{N}} + (d\ell)^{-2}$ on the space $L^2(B(u))$ extended to all of $L^2(\mathbb{R}^3)$ by letting it be 0 on the orthogonal complement, i.e., on functions that live outside $B(u)$.

Note that if $\varepsilon_T = 0$ then $\widehat{\mathcal{T}}_u$ equals $\mathcal{T}_u$. For the kinetic energy $\widehat{\mathcal{T}}_u$ we have a result similar to Corollary 3.6. For the following theorem we note that on the domain $H_0^1(\Lambda)$ we have

$$\int -\Delta_u^{\mathcal{N}} \, \mathrm{d}u = -\Delta_D \tag{43}$$

in the sense of quadratic forms.

3.7 LEMMA (Large-box kinetic energy localization)**.** *If $M \geq 5$, and $b, d, s, \varepsilon_T > 0$ are smaller than some universal constant then*

$$\int_{\mathbb{R}^3} \widehat{\mathcal{T}}_u \, \mathrm{d}u \leq -\Delta. \tag{44}$$

Proof. As usual we set $\ell = 1$. The first step in the proof is to show that for all $d > 0$

$$\int_{\mathbb{R}^3} \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + d^{-2}}\,\mathrm{d}u \leq \frac{-\Delta}{-\Delta + d^{-2}}. \tag{45}$$

To show this, we recall that in the sense of quadratic forms $\sum_{u\in\mathbb{Z}^3} -\Delta_u^{\mathcal{N}} \leq -\Delta$. Thus

$$(-\Delta + d^{-2})^{-1} \leq \left(\sum_{u\in\mathbb{Z}^3} -\Delta_u^{\mathcal{N}} + d^{-2}\right)^{-1} = \sum_{u\in\mathbb{Z}^3} (-\Delta_u^{\mathcal{N}} + d^{-2})^{-1}. \tag{46}$$

The last equality looks odd, but it is just the identity $(\bigoplus_u A_u)^{-1} = \bigoplus_u A_u^{-1}$ applied to the operators $A_u = -\Delta_u^{\mathcal{N}} + d^{-2}\mathbb{1}_{L^2(B(u))}$ acting on $L^2(B(u))$ recalling that $L^2(\mathbb{R}^3) = \bigoplus_{u\in\mathbb{Z}^3} L^2(B(u))$.

Since $1 - d^{-2}(-\Delta + d^{-2})^{-1} = -\Delta(-\Delta + d^{-2})^{-1}$, it follows from (46) that

$$\sum_{u\in\mathbb{Z}^3} \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + d^{-2}} \leq \frac{-\Delta}{-\Delta + d^{-2}}. \tag{47}$$

This will also hold if we replace the sum over $\mathbb{Z}^3$ by a sum over $v + \mathbb{Z}^3$ for any $v \in [0,1]^3$. An integration over $v \in [0,1]^3$ gives (45).

The second step is to observe that from Lemma 3.5, e.g., with $M \geq 5$ we find that

$$\begin{aligned}
&\int Q_u\chi_u \left[(1-\varepsilon_T)\left[\sqrt{-\Delta} - \tfrac{1}{2}s^{-1}\right]_+^2 + \varepsilon_T\left[\sqrt{-\Delta} - \tfrac{1}{2}(ds)^{-1}\right]_+^2\right]\chi_u Q_u\,\mathrm{d}u \\
&\leq\ (1-\varepsilon_T)\left[\sqrt{-\Delta} - \tfrac{1}{4}s^{-1}\right]_+^2 + \varepsilon_T\left[\sqrt{-\Delta} - \tfrac{1}{4}(ds)^{-1}\right]_+^2 + Cs\frac{-\Delta}{-\Delta+\beta}
\end{aligned}$$

for some universal constant C and where β is the same constant as in (40). The proof is completed using (40) and observing that if s, b, d, ε_T are all smaller than some universal constant then for all $p \in \mathbb{R}^3$

$$(b\beta^{-1} + Cs)\frac{p^2}{p^2+\beta} + \varepsilon_T d^{-2}\frac{p^2}{p^2+d^{-2}} + (1-\varepsilon_T)\left[|p| - \tfrac{1}{4}s^{-1}\right]_+^2 + \varepsilon_T\left[|p| - \tfrac{1}{4}(ds)^{-1}\right]_+^2 \leq p^2.$$

□

We now discuss the further localization into smaller boxes of relative size $d \ll 1$. As in the previous subsection we index these boxes by a parameter $u' \in \mathbb{R}^3$. The small box is $\widetilde{B}(u') = d\ell\Gamma_{u'} = d\ell u' + [-d\ell/2, d\ell/2]^3$, whose center is at $d\ell u'$. We denote the corresponding characteristic function and localization function by

$$\widetilde{\theta}_{u'}(x) = \theta((x/d\ell) - u'), \quad \widetilde{\chi}_{u'}(x) = \chi((x/d\ell) - u').$$

The corresponding orthogonal projection onto functions orthogonal to constants in $L^2(\widetilde{B}(u'))$ is $\widetilde{Q}_{u'}$ given by

$$\widetilde{Q}_{u'} f = \widetilde{\theta}_{u'} f - (d\ell)^{-3} \langle \widetilde{\theta}_{u'} | f \rangle \widetilde{\theta}_{u'}.$$

When localizing in to the smaller boxes, we are forced to consider the situation of overlap between the large boxes and small boxes, i.e., $B(u, u') = B(u) \cap \widetilde{B}(u')$. The corresponding characteristic function is $\theta_u \widetilde{\theta}_{u'}$, the corresponding localization function is $\chi_u \widetilde{\chi}_{u'}$, and the corresponding orthogonal projection is

$$Q_{uu'} f = \theta_u \widetilde{\theta}_{u'} f - |B(u, u')|^{-1} \langle \theta_u \widetilde{\theta}_{u'} | f \rangle \theta_u \widetilde{\theta}_{u'}.$$

Our first result is that when we localize the large box kinetic energy $\widehat{\mathcal{T}}_u$ into smaller boxes we will get a gap in the localized energy spectrum. This is a consequence of the next result.

3.8 LEMMA. *With $Q_{uu'}$ as defined above and $\widetilde{\beta} = 1 + \pi^{-2}$ we have for all $d > 0$*

$$\int Q_{uu'} \, \mathrm{d}u' \leq \widetilde{\beta} \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + (d\ell)^{-2}}. \tag{48}$$

Proof. It is enough to consider $\ell = 1$. Let $-\Delta_{uu'}^{\mathcal{N}}$ denote the Neumann Laplacian in the box $B(u, u')$. Observe that since $B(u, u') \subseteq \widetilde{B}(u')$, the Neumann Laplacian $-\Delta_{uu'}^{\mathcal{N}}$ has a gap of at least $\pi^2 d^{-2}$, i.e., $-\Delta_{uu'}^{\mathcal{N}} \geq \pi^2 d^{-2} Q_{uu'}$. Thus

$$Q_{uu'} \leq \widetilde{\beta} \frac{-\Delta_{uu'}^{\mathcal{N}}}{-\Delta_{uu'}^{\mathcal{N}} + d^{-2}}.$$

The same argument that led to (45) gives

$$\int \frac{-\Delta_{uu'}^{\mathcal{N}}}{-\Delta_{uu'}^{\mathcal{N}} + d^{-2}} \, \mathrm{d}u' \leq \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + d^{-2}},$$

which concludes the proof of the lemma. □

This lemma shows that the first term in (42), after localization, leads to a gap in the small boxes. The full kinetic energy localization is given in the next lemma.

3.9 LEMMA (Small-box kinetic energy localization)**.** *Let $\widehat{\mathcal{T}}_u$ be the kinetic energy given in*

(42) in terms of the parameters s, d, ε_T and the constant b. Let

$$\mathcal{T}_{uu'} = \varepsilon_T \widetilde{b}(d\ell)^{-2} Q_{uu'} + Q_{uu'}\chi_u\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds\ell)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\chi_u Q_{uu'}. \tag{49}$$

Our assertion is that if $(s^{-2}+d^{-3})(ds)^{-2}s^M \le \delta$, then, for all $0 < \varepsilon_T < 1$,

$$\widehat{\mathcal{T}}_u - \frac{b}{2}\ell^{-2}Q_u \ge \int \mathcal{T}_{uu'}\,\mathrm{d}u',$$

provided that $\widetilde{b}$ and d are smaller than some universal constant. The first term in (49) yields a gap above zero of size $\varepsilon_T\widetilde{b}(d\ell)^{-2}$ in the spectrum of $\mathcal{T}_{uu'}$, which we will refer to as the Neumann gap.

Proof. We again take $\ell = 1$. The integral over the first term in $\mathcal{T}_{uu'}$ is bounded above by the first term in $\widehat{\mathcal{T}}_u$ by Lemma 3.8 if $\widetilde{b}$ is smaller than the constant $\widetilde{\beta}^{-1}$ in that lemma. We concentrate on the second term in $\mathcal{T}_{uu'}$. By a unitary transformation ($x \mapsto x/d$ and $p \mapsto pd$) of the result in Lemma 3.5 we obtain that

$$\begin{aligned}
&\int \widetilde{Q}_{u'}\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\widetilde{Q}_{u'}\,\mathrm{d}u' \le d^{-2}F_s(d\sqrt{-\Delta})\\
&\le\ (1-\varepsilon_T)\left[\sqrt{-\Delta} - \tfrac{1}{2}s^{-1}\right]_+^2 + \varepsilon_T\left[\sqrt{-\Delta} - \tfrac{1}{2}(ds)^{-1}\right]_+^2 + C(ds)^{-2}s^{M-2},
\end{aligned}$$

where the function F_s is given in (35) and we used that $\left[\sqrt{-\Delta} - \frac{1}{2}(ds)^{-1}\right]_+^2 \le \left[\sqrt{-\Delta} - \frac{1}{2}s^{-1}\right]_+^2$. Thus the proof would be complete if the operator appearing as the integrand in the second term in $\mathcal{T}_{uu'}$ would have been, instead,

$$Q_u\chi_u\widetilde{Q}_{u'}\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\widetilde{Q}_{u'}\chi_u Q_u.$$

We will estimate the difference between these operators, which is

$$\begin{aligned}
D\ &=\ Q_u\chi_u\widetilde{Q}_{u'}\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\widetilde{Q}_{u'}\chi_u Q_u\\
&\quad -Q_{uu'}\chi_u\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\chi_u Q_{uu'}\\
&=\ Q_u\left(\chi_u\widetilde{Q}_{u'} - Q_{uu'}\chi_u\right)\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\widetilde{Q}_{u'}\chi_u Q_u\\
&\quad +Q_{uu'}\chi_u\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2 \widetilde{\chi}_{u'}\left(\widetilde{Q}_{u'}\chi_u - \chi_u Q_{uu'}\right)Q_u,
\end{aligned}$$

where we have used that $Q_u Q_{uu'} = Q_{uu'}$. We observe that (using Dirac notation)

$$\begin{aligned}\left(\chi_u \widetilde{Q}_{u'} - Q_{uu'}\chi_u\right)\widetilde{\chi}_{u'} &= \chi_u\widetilde{\theta}_{u'}\widetilde{\chi}_{u'} - d^{-3}\chi_u|\widetilde{\theta}_{u'}\rangle\langle\widetilde{\theta}_{u'}|\widetilde{\chi}_{u'} - \theta_u\widetilde{\theta}_{u'}\chi_u\widetilde{\chi}_{u'} \\ &\quad + |B(u,u')|^{-1}|\theta_u\widetilde{\theta}_{u'}\rangle\langle\theta_u\widetilde{\theta}_{u'}|\chi_u\widetilde{\chi}_{u'} \\ &= |B(u,u')|^{-1}|\theta_u\widetilde{\theta}_{u'}\rangle\langle\chi_u\widetilde{\chi}_{u'}| - d^{-3}|\chi_u\widetilde{\theta}_{u'}\rangle\langle\widetilde{\chi}_{u'}|,\end{aligned}$$

exploiting the facts that $\widetilde{\theta}_{u'}\widetilde{\chi}_{u'} = \widetilde{\chi}_{u'}$ and $\theta_u\chi_u = \chi_u$. It is now simple to estimate the operator norm of D

$$\begin{aligned}\|D\| &\leq C\left\|\left(\chi_u\widetilde{Q}_{u'} - Q_{uu'}\chi_u\right)\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2\right\| \\ &\leq C|B(u,u')|^{-1/2}\left(\int_{|p|>(ds)^{-1}} |p|^4\,|\widehat{\chi_u\widetilde{\chi}_{u'}}(p)|^2\,\mathrm{d}p\right)^{1/2} \\ &\quad + Cd^{-3/2}\left(\int_{|p|>(ds)^{-1}} |p|^4\,|\widehat{\widetilde{\chi}_{u'}}(p)|^2\,\mathrm{d}p\right)^{1/2} \\ &\leq C(ds)^{M-2}|B(u,u')|^{-1/2}\langle\chi_u\widetilde{\chi}_{u'}|(-\Delta)^M\chi_u\widetilde{\chi}_{u'}\rangle^{1/2} + C(ds)^{M-2}d^{-3/2}\langle\widetilde{\chi}_{u'}|(-\Delta)^M\widetilde{\chi}_{u'}\rangle^{1/2} \\ &\leq C(ds)^{M-2}d^{-M} \leq C(ds)^{-2}s^M.\end{aligned}$$

Hence $D = Q_u D Q_u \geq -C(ds)^{-2}s^M Q_u$ and

$$\begin{aligned}&\int Q_{uu'}\chi_u\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2\widetilde{\chi}_{u'}\chi_u Q_{uu'}\,\mathrm{d}u' \\ &= \int Q_u\chi_u\widetilde{Q}_{u'}\widetilde{\chi}_{u'}\left[\sqrt{-\Delta} - (ds)^{-1}\right]_+^2\widetilde{\chi}_{u'}\widetilde{Q}_{u'}\chi_u Q_u\,\mathrm{d}u' - \int_{\{u'|B(u)\cap\widetilde{B}(u')\neq\emptyset\}} D\,\mathrm{d}u' \\ &\leq Q_u\chi_u\left((1-\varepsilon_T)\left[\sqrt{-\Delta} - \tfrac{1}{2}s^{-1}\right]_+^2 + \varepsilon_T\left[\sqrt{-\Delta} - \tfrac{1}{2}(ds)^{-1}\right]_+^2\right)\chi_u Q_u \\ &\quad + C(s^{-2} + d^{-3})(ds)^{-2}s^M Q_u.\end{aligned}$$

We have here used the fact that the volume of $\{u'|B(u)\cap\widetilde{B}(u')\neq\emptyset\}$ is bounded by Cd^{-3}. □

We shall throughout the rest of the paper assume that the conditions in Lemmas 3.7 and 3.9 are satisfied.

CONDITION 2: *In terms of the integer M appearing in the definition (16) of χ (and which will be specified later to be ≥ 5) we have*

$$0 < \varepsilon_T < \delta, \quad \textit{and} \quad (s^{-2} + d^{-3})(ds)^{-2}s^M \leq \delta, \tag{50}$$

where δ is the quantity which we introduced in Condition 1 to ensure adequate smallness of *relevant parameters.*

3.3 Localization of the Total Energy

We define the localized Hamiltonian, H_u, in a "large" box $B(u)$ to be

$$\begin{aligned} H_u &= \sum_{i=1}^{N}\left((1-\varepsilon_0)\widehat{\mathcal{T}}_{u,i} - \rho\int w_{B(u)}(x_i,y)\,\mathrm{d}y\right) + \sum_{1\le i<j\le N} w_{B(u)}(x_i,x_j) \\ &\quad + \frac{1}{2}\rho^2\iint w_{B(u)}(x,y)\,\mathrm{d}x\,\mathrm{d}y, \end{aligned} \tag{51}$$

where $0 < \varepsilon_0 < 1/2$ is a parameter to be determined later. The subscript i, as usual, refers to the i^{th} particle. Recall that $\widehat{\mathcal{T}}_u$ was defined in (42) and $w_{B(u)}$ was defined in (24). The Hamiltonian H_u is defined as a quadratic form on permutation-symmetric functions in $H_0^1(\Lambda^N)$.

The localized Hamiltonian in a "small" box $B(u,u')$ is

$$\begin{aligned} H_{uu'} &= \sum_{i=1}^{N}\left((1-\varepsilon_0)\mathcal{T}_{uu',i} - \rho\int w_{B(u,u')}(x_i,y)\,\mathrm{d}y\right) + \sum_{1\le i<j\le N} w_{B(u,u')}(x_i,x_j) \\ &\quad + \frac{1}{2}\rho^2\iint w_{B(u,u')}(x,y)\,\mathrm{d}x\,\mathrm{d}y, \end{aligned} \tag{52}$$

where $w_{B(u,u')}$ was defined in (24) and $\mathcal{T}_{uu'}$ was defined in (49). The results of Proposition 3.1, (43) and Lemmas 3.7 and 3.9 can be combined to give our final localization estimate.

3.10 THEOREM (Main localization inequalities)**.**
If Condition 2 is satisfied, we have for all $0 \le \varepsilon_0 \le 1/2$ *that*

$$H_{\rho,N} \ge \int_{\ell^{-1}\Lambda'}\left(-\varepsilon_0\Delta_u^{\mathcal{N}} + H_u\right)\mathrm{d}u, \quad \textit{and, for all } u\in\mathbb{R}^3, \quad H_u - \frac{b}{2}\ell^{-2}Q_u \ge \int_{\mathbb{R}^3} H_{uu'}\,\mathrm{d}u'. \tag{53}$$

We introduce the notation that

$$H_B = \begin{cases} H_u, & \text{if } B = B(u) \\ H_{uu'}, & \text{if } B = B(u,u') \end{cases} \tag{54}$$

and

$$\mathcal{T}_B = \begin{cases} (1-\varepsilon_0)\widehat{\mathcal{T}}_u, & \text{if } B = B(u) \\ (1-\varepsilon_0)\mathcal{T}_{uu'}, & \text{if } B = B(u,u'). \end{cases} \tag{55}$$

The reason for the above $(1-\varepsilon_0)$ term is that we still need some kinetic energy in the end of this paper when we want to apply Lemma 6.6. With the corresponding notations for w_B in (24) the box Hamiltonian can be written

$$H_B = \sum_{i=1}^{N}\left(\mathcal{T}_{B,i} - \rho\int w_B(x_i,y)\,\mathrm{d}y\right) + \sum_{1\le i<j\le N} w_B(x_i,x_j) + \frac{1}{2}\rho^2\iint w_B(x,y)\,\mathrm{d}x\,\mathrm{d}y. \quad (56)$$

4 Energy in a Single Box

In this section we will study the energy in a single box B, i.e., the ground state energy of the Hamiltonian H_B. We denote by P_B the orthogonal projection onto the characteristic function of B and by Q_B the projection orthogonal to constant functions in B, i.e., such that $P_B + Q_B = \mathbb{1}_B$ is the projection onto the subspace of functions supported on B. We define the operators

$$n = \sum_{i=1}^{N}\mathbb{1}_{B,i}, \quad n_0 = \sum_{i=1}^{N} P_{B,i}, \quad n_+ = \sum_{i=1}^{N} Q_{B,i}.$$

Here n represents the number of particles in the box B, n_0 the number of particles in the constant function, which we will refer to as the *condensate particles*, and n_+ the number of particles not in the condensate, which we will refer to as the *excited particles*. We have $n = n_+ + n_0$.

The particle number operator n commutes with the box operator H_B, but n_+ and n_0 do not commute with H_B. In our discussion below we may assume that n is a parameter, i.e., we restrict to eigenspaces for the operator n. We shall not distinguish between the operator n and its eigenvalues.

We give a simple a priori bound on n_+, which will be improved later.

4.1 LEMMA (Simple bound on the ground state energy of H_B and on n_+).
The ground state energy E_B of H_B satisfies

$$0 > E_B \geq -Cn\rho|B|\mathcal{U}_B \quad (57)$$

with $\mathcal{U}_B$ given in (25). Moreover, in any state for which the expectation value $\langle H_B\rangle \leq \frac{1}{2}\rho^2\iint w_B(x,y)\,\mathrm{d}x\,\mathrm{d}y = \rho^2|B|^2\mathcal{U}_B$ we have

$$\langle n_+\rangle \leq C(1-\varepsilon_0)^{-1}\varepsilon_T^{-1}\widetilde{b}^{-1}\rho a(d\ell)^2 n \max\chi_B^2, \quad (58)$$

if $B = B(u, u')$.

Proof. The upper bound on E_B follows by using a trial state in which all particles are in the condensate, i.e., an eigenstate of n_+ with eigenvalue 0. If there are n particles, we find that the expectation value in this state is

$$\langle H_B \rangle = \frac{1}{2}\left[(n - \rho|B|)^2 - n\right] |B|^{-2} \iint w_B(x, y)\,\mathrm{d}x\,\mathrm{d}y.$$

We can choose $n \geq 1$ such that $|n - \rho|B|| < 1$. Hence $\langle H_B \rangle < 0$ and thus the ground state energy of H_B is negative. The lower bound on E_B follows immediately from (26) since $\mathcal{T}_B$ and w_B are non-negative.

If a state satisfies $\langle H_B \rangle \leq \frac{1}{2}\rho^2 \iint w_B(x, y)\,\mathrm{d}x\,\mathrm{d}y$, we have

$$0 \;\geq\; \sum_{i=1}^{N} \left\langle \mathcal{T}_{B,i} - \rho \int w_B(x_i, y)\,\mathrm{d}y \right\rangle \geq (1 - \varepsilon_0)\varepsilon_T \widetilde{b}(d\ell)^{-2}\langle n_+ \rangle - C\rho a n \max \chi_B^2,$$

where we have used (49) and that $\max_x \int \omega_B(x, y)\,\mathrm{d}y \leq Ca \max \chi_B^2$ as we have seen in Lemma 3.2. This gives the second estimate in the lemma. □

4.1 The Negligible (Non-Quadratic) Parts of the Potential

We treat the potential energy terms in H_B according to how many excited particles they involve. We write $\mathbb{1}_B = P_B + Q_B$ and we expand and classify the terms according to the number of Q-factors, no-Q, 1-Q, ..., 4-Q. In the following we will simply write $P_B = P$ and $Q_B = Q$.

no-$\mathcal{Q}$ terms:

$$\begin{aligned}\mathcal{Q}_0 \;&:=\; -\sum_i \rho P_i \int w_B(x_i, y)\,\mathrm{d}y P_i + \sum_{i<j} P_i P_j w_B(x_i, x_j) P_i P_j + \frac{1}{2}\rho^2 \iint w_B(x, y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \;\left[(n_0 - \rho|B|)^2 - n_0\right] \mathcal{U}_B = \left[(n - \rho|B|)^2 - 2(n - \rho|B|)n_+ + n_+^2 - n_0\right] \mathcal{U}_B, \qquad (59)\end{aligned}$$

where we have used the notation (25).

1-$\mathcal{Q}$ terms:

$$\mathcal{Q}_1 \;:=\; \sum_{i,j} P_i P_j w_B(x_i, x_j) Q_i P_j - \sum_i \rho P_i \int w_B(x_i, y)\,\mathrm{d}y Q_i + \text{h.c.}$$

$$
\begin{aligned}
&= \sum_i P_i \int w_B(x_i, y)\,\mathrm{d}y Q_i (n_0|B|^{-1} - \rho) + \text{h.c.} \\
&= \mathcal{Q}_1' + \mathcal{Q}_1'', \qquad (60)
\end{aligned}
$$

where

$$
\mathcal{Q}_1' = (n - \rho|B|)|B|^{-1}\left(\sum_i P_i \int w_B(x_i, y)\,\mathrm{d}y Q_i + \sum_i Q_i \int w_B(x_i, y)\,\mathrm{d}y P_i\right) \qquad (61)
$$

and

$$
\mathcal{Q}_1'' = -|B|^{-1}\sum_i P_i \int w_B(x_i, y)\,\mathrm{d}y Q_i n_+ - |B|^{-1}\sum_i n_+ Q_i \int w_B(x_i, y)\,\mathrm{d}y P_i. \qquad (62)
$$

4.2 LEMMA (Estimates on $\mathcal{Q}_1$)**.** *For all* $\varepsilon_1', \varepsilon_1'' > 0$

$$
\mathcal{Q}_1' \geq -\,|n - \rho|B||(\varepsilon_1' n_0 + \varepsilon_1'^{-1} C n_+)\mathcal{U}_B
$$

and

$$
\mathcal{Q}_1'' \geq -\,(\varepsilon_1''(n_+ + 1)n_0 + C\varepsilon_1''^{-1} n_+^2)\,\mathcal{U}_B.
$$

Proof. We prove first the bound on $\mathcal{Q}_1''$. We have

$$
\mathcal{Q}_1'' = -\sqrt{n_+ + 1}\sum_i P_i \int w_B(x_i, y)\,\mathrm{d}y Q_i \sqrt{n_+}\,|B|^{-1} + \text{h.c.}
$$

since for any self-adjoint operator A we get $\sum_i P_i A_i Q_i n_+ = (n_+ + 1)\sum_i P_i A_i Q_i$ and hence $\sum_i P_i A_i Q_i \sqrt{n_+} = \sqrt{n_+ + 1}\sum_i P_i A_i Q_i$.

Since $w_B \geq 0$, we obtain from a Schwarz inequality and Lemma 3.2 that

$$
\mathcal{Q}_1'' \geq -\left(\varepsilon_1''(n_+ + 1)\sum_i P_i + C\varepsilon_1''^{-1} n_+ \sum_i Q_i\right)\mathcal{U}_B.
$$

The estimate on $\mathcal{Q}_1'$ follows by applying a similar Schwarz inequality. □

2-$\mathcal{Q}$ terms: There are two kinds of 2-$\mathcal{Q}$ terms. There are terms which contribute to the energy to the order of interest. They will primarily be treated together with the quadratic Hamiltonian later on. The remaining 2-$\mathcal{Q}$ terms are negligible error terms that we will estimate here.

The 2-$\mathcal{Q}$ terms that will later appear in the quadratic Hamiltonian are

$$\mathcal{Q}_2' := \sum_{i,j} P_iQ_jw_B(x_i,x_j)P_jQ_i + \sum_{i<j}(Q_iQ_jw_B(x_i,x_j)P_jP_i + P_jP_iw_B(x_i,x_j)Q_iQ_j). \quad (63)$$

We shall however give an a priori estimate on these terms already now. This estimate will be used in Case II in the proof of Lemma 5.2. Using the estimate $0 \le w_B \le CaR^{-3}\max\chi_B^2$ and the Schwarz inequality twice gives that

$$\begin{aligned}
\mathcal{Q}_2' &\ge -\sum_{i,j} P_iQ_jw_B(x_i,x_j)P_iQ_j - \sum_{i<j}\left(2Q_iQ_jw_B(x_i,x_j)Q_jQ_i + \frac{1}{2}P_jP_iw_B(x_i,x_j)P_iP_j\right) \\
&\ge -n_0|B|^{-1}\sum_i Q_i\int w_B(x_i,y)\,\mathrm{d}yQ_i - Cn_+^2aR^{-3}\max\chi_B^2 - \frac{1}{2}\sum_{i<j}P_jP_iw_B(x_i,x_j)P_iP_j \\
&\ge -Cnn_+\mathcal{U}_B - Cn_+^2aR^{-3}\max\chi_B^2 - \frac{1}{2}n^2\mathcal{U}_B. \qquad (64)
\end{aligned}$$

In the last inequality we have used that $\sum_i Q_i\int\omega_B(x_i,y)\,\mathrm{d}yQ_i \le C|B|\mathcal{U}_Bn_+$ by (26) since $\sum_i Q_i\int\omega_B(x_i,y)\,\mathrm{d}yQ_i$ commutes with n_+. The negligible 2-$\mathcal{Q}$ terms are estimated in the same way

$$\begin{aligned}
\mathcal{Q}_2'' &:= -\sum_i \rho Q_i\int w_B(x_i,y)\,\mathrm{d}yQ_i + \sum_{i,j} Q_iP_jw_B(x_i,x_j)P_jQ_i \\
&= (n_0-\rho|B|)|B|^{-1}\sum_i Q_i\int w_B(x_i,y)\,\mathrm{d}yQ_i \qquad (65) \\
&= (n-\rho|B|-n_+)|B|^{-1}\sum_i Q_i\int w_B(x_i,y)\,\mathrm{d}yQ_i \ge -C\left([\rho|B|-n]_+n_+ + n_+^2\right)\mathcal{U}_B.
\end{aligned}$$

3-$\mathcal{Q}$ terms: For all $\varepsilon_3 > 0$

$$\begin{aligned}
\mathcal{Q}_3 &:= \sum_{i,j} P_jQ_iw_B(x_i,x_j)Q_iQ_j + \text{ h.c.} \\
&\ge -\sum_{i\ne j}\left(2\varepsilon_3^{-1}P_jQ_iw_B(x_i,x_j)Q_iP_j + \frac{\varepsilon_3}{2}Q_jQ_iw_B(x_i,x_j)Q_iQ_j\right) \\
&\ge -C\varepsilon_3^{-1}nn_+\mathcal{U}_B - \varepsilon_3\sum_{i<j}Q_jQ_iw_B(x_i,x_j)Q_iQ_j. \qquad (66)
\end{aligned}$$

The first inequality uses a Schwarz inequality, while the second inequality uses Lemma 3.2 and the fact that $n_0 \le n$. Note that the above estimates are given as lower bounds, but that we of course also could have stated them as two-sided bounds. The last term above can be absorbed into the positive 4-$\mathcal{Q}$ term if $\varepsilon_3 \leq 1$. We will do this initially, but at a later stage in the proof we have to control the first term in (66) by choosing $\varepsilon_3 \gg 1$. At that time we will have good control over the number of excited particles, n_+, in the large box. The second term in (66) will then be controlled by applying Lemma 6.6, where we apply the kinetic energy term $\sum_i -\varepsilon_0 \Delta_{u,i}^{\mathcal{N}}$ that we have saved in Theorem 3.10 for exactly this purpose.

4-$\mathcal{Q}$ term: This is the positive term

$$\mathcal{Q}_4 := \sum_{i<j} Q_j Q_i w_B(x_i, x_j) Q_i Q_j \tag{67}$$

and for a lower bound it can be ignored or used to control other errors. We will only need an estimate on the 4-$\mathcal{Q}$ term in a large box $B = B(u)$ as explained above.

4.2 The Quadratic Hamiltonian

We can write the box Hamiltonian as

$$H_B = \sum_{i=1}^{N} \mathcal{T}_{B,i} + \mathcal{Q}_0 + \mathcal{Q}_1' + \mathcal{Q}_1'' + \mathcal{Q}_2' + \mathcal{Q}_2'' + \mathcal{Q}_3 + \mathcal{Q}_4. \tag{68}$$

We have estimated all terms except the *quadratic part* $\sum_{i=1}^{N} \mathcal{T}_{B,i} + \mathcal{Q}_2'$. We first consider the kinetic energy.

For $B = B(u)$, i.e., a large box we have from (42) and (55) that

$$\mathcal{T}_B = (1-\varepsilon_0)\varepsilon_T (d\ell)^{-2} \frac{-\Delta_u^{\mathcal{N}}}{-\Delta_u^{\mathcal{N}} + (d\ell)^{-2}} + (1-\varepsilon_0) b\ell^{-2} Q + Q\chi_B \tau_B(-\Delta)\chi_B Q \tag{69}$$

with

$$\tau_B(k^2) = (1-\varepsilon_0)(1-\varepsilon_T)\ \left[|k| - \tfrac{1}{2}(s\ell)^{-1}\right]_+^2\ + (1-\varepsilon_0)\varepsilon_T\ \left[|k| - \tfrac{1}{2}(ds\ell)^{-1}\right]_+^2. \tag{70}$$

For $B = B(u, u')$, i.e., a small box we have from (49) and (55) that

$$\mathcal{T}_B = (1-\varepsilon_0)\varepsilon_T \widetilde{b} (d\ell)^{-2} Q + Q\chi_B \tau_B(-\Delta)\chi_B Q \tag{71}$$

with

$$\tau_B(k^2) = (1-\varepsilon_0)\left[|k| - (ds\ell)^{-1}\right]_+^2. \tag{72}$$

The interesting part of $\mathcal{T}_B$ is the term of form $Q\chi_B\tau_B(-\Delta)\chi_B Q$. The other terms, which are positive, are only used to control errors. We put them aside for the moment and define the *quadratic Hamiltonian*

$$H_{\rm Quad} = \sum_{i=1}^{N} (Q\chi_B\tau_B(-\Delta)\chi_B Q)_i + \mathcal{Q}_2'. \tag{73}$$

At the end of this paper it will be useful to treat the term $\mathcal{Q}_1'$ together with $H_{\rm Quad}$.
To handle $H_{\rm Quad}$, we use the formalism of second quantization. For all $k \in \mathbb{R}^3$ we define the operator

$$b_k = a_0^* a(Q(e^{ikx}\chi_B)), \tag{74}$$

where $a(Q(e^{ikx}\chi_B))$ is the operator that annihilates an exited particle in the state given by the function $Q(e^{ikx}\chi_B) \in L^2(B)$, and a_0 is the operator that creates a particle in the condensate. These two operators commute. Note that b_k is a bounded operator when restricted to a subspace of finite n. Its adjoint is

$$b_k^* = a(Q(e^{ikx}\chi_B))^* a_0. \tag{75}$$

Since a_0^* commutes with $a(Q(e^{ikx}\chi_B))$, we have the commutation relations

$$[b_k, b_{k'}] = 0, \quad [b_k, b_{k'}^*] = a_0^* a_0 \big\langle Q(e^{ikx}\chi_B) \big| Q(e^{ik'x}\chi_B) \big\rangle - a(Q(e^{ik'x}\chi_B))^* a(Q(e^{ikx}\chi_B)), \tag{76}$$

for all $k, k' \in \mathbb{R}^3$. In particular,

$$[b_k, b_k^*] \le a_0^* a_0 \int \chi_B^2 = n_0 \int \chi_B^2. \tag{77}$$

Moreover,

$$b_k^* b_k \le n_+(n_0+1) \int \chi_B^2. \tag{78}$$

The term $Q\chi_B\tau_B(-\Delta)\chi_B Q$ and its second quantization can be written

$$\begin{aligned}
Q\chi_B\tau_B(-\Delta)\chi_B Q &= (2\pi)^{-3} \int_{\mathbb{R}^3} \tau_B(k^2) \left| Q(\chi_B e^{ikx}) \right\rangle \left\langle Q(\chi_B e^{ikx}) \right| \, \mathrm{d}k \\
&\xrightarrow{2^{\rm nd}\text{ quant}} (2\pi)^{-3} \int_{\mathbb{R}^3} \tau_B(k^2) a(Q(\chi_B e^{ikx}))^* a(Q(\chi_B e^{ikx}))\, \mathrm{d}k \\
&\ge (2\pi)^{-3} \int_{\mathbb{R}^3} \tau_B(k^2) a(Q(\chi_B e^{ikx}))^* \frac{a_0 a_0^*}{n} a(Q(\chi_B e^{ikx}))\, \mathrm{d}k \\
&= (2\pi)^{-3} n^{-1} \int_{\mathbb{R}^3} \tau_B(k^2) b_k^* b_k \, \mathrm{d}k.
\end{aligned} \tag{79}$$

Here we used that $b_k\psi = 0$ if ψ is in the condensate allowing us to assume that $n_+ \geq 1$ such that in fact $a_0 a_0^* \leq n$. Likewise we may write

$$\begin{aligned} \mathcal{Q}_2' &= \frac{1}{2}(2\pi)^{-3}|B|^{-1}\int \widehat{W}(k)\left(b_k^* b_k + b_{-k}^* b_{-k} + b_k^* b_{-k}^* + b_k b_{-k}\right)\,\mathrm{d}k \\ &\quad -(2\pi)^{-3}|B|^{-1}\int \widehat{W}(k) a(Q(\chi_B e^{ikx}))^* a(Q(\chi_B e^{ikx}))\,\mathrm{d}k \end{aligned} \tag{80}$$

and

$$\mathcal{Q}_1' = (n-\rho|B|)(2\pi)^{-3}|B|^{-3/2}\int \widehat{W}(k)\left(\overline{\widehat{\chi}_B(k)}b_k + \widehat{\chi}_B(k)b_k^*\right)\,\mathrm{d}k. \tag{81}$$

The last term in $\mathcal{Q}_2'$ may be written

$$(2\pi)^{-3}|B|^{-1}\int \widehat{W}(k) a(Q(\chi_B e^{ikx}))^* a(Q(\chi_B e^{ikx}))\,\mathrm{d}k = \sum_{i=1}^N Q_i Z_i Q_i, \tag{82}$$

where Z is the operator with integral kernel

$$k_Z(x,y) = |B|^{-1}\chi_B(x)W(x-y)\chi_B(y). \tag{83}$$

4.3 LEMMA. *The operator Z on $L^2(\mathbb{R}^3)$ with integral kernel (83) satisfies the bound*

$$\|Z\| \leq Ca\min\{R^{-3}, |B|^{-1}\}\max\chi_B^2.$$

In particular, if $B = B(u)$, we have

$$||Z|| \leq Ca|B|^{-1}. \tag{84}$$

Proof. It is clear that

$$\|Z\| \leq |B|^{-1}\max\chi_B^2\int W \leq C|B|^{-1}\max\chi_B^2\int v_1 \leq Ca|B|^{-1}\max\chi_B^2.$$

If we use that the Hilbert-Schmidt norm is greater than the operator norm, $\|Z\| \leq \|Z\|_{\mathrm{HS}}$, we find

$$\|Z\| \leq |B|^{-1}\left(\iint \chi_B(x)^2 W(x-y)^2\chi_B(y)^2\,\mathrm{d}x\,\mathrm{d}y\right)^{1/2} \leq |B|^{-1}\max W\int \chi_B^2 \leq CaR^{-3}\max\chi_B^2.$$

□

Combining the above lemma with (73), (79), (80), and (81), we arrive at the following result.

4.4 LEMMA. *For all $\sigma \in \mathbb{R}$ we have the estimate*

$$H_{\mathrm{Quad}} + \sigma \mathcal{Q}_1' \geq \frac{1}{2}(2\pi)^{-3} \int_{\mathbb{R}^3} h_\sigma(k)\,\mathrm{d}k - Cn_+ a \min\{R^{-3}, |B|^{-1}\} \max \chi_B^2, \tag{85}$$

where

$$\begin{aligned} h_\sigma(k) &= n^{-1}\tau_B(k^2)(b_k^* b_k + b_{-k}^* b_{-k}) + \widehat{W}(k)|B|^{-1}(b_k^* b_k + b_{-k}^* b_{-k} + b_k^* b_{-k}^* + b_k b_{-k}) \\ &\quad + \sigma(n - \rho|B|)\widehat{W}(k)|B|^{-3/2}\left(\overline{\widehat{\chi}_B(k)}(b_k + b_{-k}^*) + \widehat{\chi}_B(k)(b_k^* + b_{-k})\right). \end{aligned}$$

(If $n = 0$ then $h_\sigma(k) = 0$.)

Note that if we for the smallest side length of a small box have $\lambda_1 \geq \rho^{-\frac{1}{3}}$, then $Cn_+ a \min\{R^{-3}, |B|^{-1}\} \max \chi_B^2 \leq Cn_+ \rho a$, which is smaller than the Neumann gap on the small box.

We shall now give an estimate on $h_\sigma(k)$, which is based on a simple version of Bogolubov's treatment of quadratic Hamiltonians. This estimate requires, however, assumptions which will not be fulfilled in all our situations. The following result is Theorem 6.3 in [13] except that we state it here a bit more generally. In the original [13] it was required $\mathcal{A} \geq \mathcal{B} > 0$, but this is not needed. The operators $b_\pm$ can, for example, be any commuting pair of bounded operators (the case we will use here) or they can be annihilation operators in Fock space (the original Bogolubov case).

4.5 THEOREM (Simple case of Bogolubov's method)**.**
For arbitrary $\mathcal{A}, \mathcal{B} \in \mathbb{R}$ satisfying $\mathcal{A} > 0$, $-\mathcal{A} < \mathcal{B} \leq \mathcal{A}$ and $\kappa \in \mathbb{C}$ we have the operator inequality

$$\begin{aligned} &\mathcal{A}(b_+^* b_+ + b_-^* b_-) + \mathcal{B}(b_+^* b_-^* + b_+ b_-) + \kappa(b_+^* + b_-) + \overline{\kappa}(b_+ + b_-^*) \\ &\quad \geq -\tfrac{1}{2}(\mathcal{A} - \sqrt{\mathcal{A}^2 - \mathcal{B}^2})([b_+, b_+^*] + [b_-, b_-^*]) - \frac{2|\kappa|^2}{\mathcal{A} + \mathcal{B}}, \end{aligned}$$

where $b_\pm$ are operators on a Hilbert space satisfying $[b_+, b_-] = 0$.

Proof. The proof is essentially the same as in the original [13]. We may complete the square

$$\begin{aligned} &\mathcal{A}(b_+^* b_+ + b_-^* b_-) + \mathcal{B}(b_+^* b_-^* + b_+ b_-) + \kappa(b_+^* + b_-) + \overline{\kappa}(b_+ + b_-^*) \\ &= D(b_+^* + \alpha b_- + \overline{a})(b_+ + \alpha b_-^* + a) + D(b_-^* + \alpha b_+ + a)(b_- + \alpha b_+^* + \overline{a}) \end{aligned}$$

$$- D\alpha^2([b_+, b_+^*] + [b_-, b_-^*]) - 2D|a|^2$$

if

$$D(1+\alpha^2) = \mathcal{A}, \qquad 2D\alpha = \mathcal{B}, \qquad aD(1+\alpha) = \kappa.$$

Hence $\frac{\mathcal{B}}{\mathcal{A}}\alpha^2 - 2\alpha + \frac{\mathcal{B}}{\mathcal{A}} = 0$. If $\mathcal{B} \neq 0$, we choose the solution $\alpha = \frac{\mathcal{A}}{\mathcal{B}}\big(1 - \sqrt{1 - \frac{\mathcal{B}^2}{\mathcal{A}^2}}\,\big)$ and otherwise we choose $\alpha = 0$. Then

$$D\alpha^2 = \mathcal{B}\alpha/2 = \frac{1}{2}(\mathcal{A} - \sqrt{\mathcal{A}^2 - \mathcal{B}^2}), \qquad D|a|^2 = \frac{|\kappa|^2}{D(1+\alpha^2+2\alpha)} = \frac{|\kappa|^2}{\mathcal{A}+\mathcal{B}}.$$

□

When applying Theorem 4.5 with $\kappa = 0$, we can replace $\mathcal{B}$ by $-\mathcal{B}$, even if $\mathcal{B} = \mathcal{A}$, without changing the lower bound. This is easily seen by replacing $b_\pm$ by $\pm i b_\pm$. Hence

$$|\mathcal{B}(b_+^* b_-^* + b_+ b_-)| \leq \mathcal{A}(b_+^* b_+ + b_-^* b_-) + \tfrac{1}{2}(\mathcal{A} - \sqrt{\mathcal{A}^2 - |\mathcal{B}|^2})([b_+, b_+^*] + [b_-, b_-^*]), \tag{86}$$

which we will use on page 46. When applying this theorem to estimate $h_\sigma(k)$, we will take $b_+ = b_k$, $b_- = b_{-k}$, restricted to the appropriate n-particle sector,

$$\mathcal{A} = n^{-1}\tau_B(k^2) + \widehat{W}(k)|B|^{-1}, \quad \mathcal{B} = \widehat{W}(k)|B|^{-1}, \quad \kappa = \sigma(n - \rho|B|)\widehat{W}(k)|B|^{-3/2}\widehat{\chi}_B(k). \tag{87}$$

This choice of $\mathcal{A}$ and $\mathcal{B}$ does not necessarily satisfy the conditions in Theorem 4.5. We will now give conditions for when these are satisfied. We first observe that $\widehat{W}(0) = \int W(x)\,\mathrm{d}x > 0$ and thus

$$\widehat{W}(k) = \int \cos(kx)W(x)\,\mathrm{d}x \geq \int (1 - \frac{1}{2}(kx)^2)W(x)\,\mathrm{d}x > 0 \tag{88}$$

if $|k| < R^{-1}$ (using that W has the same range as v_R, i.e., R). Hence $\mathcal{B} > 0$ for these values of k, and the conditions in the theorem are satisfied since $\tau_B \geq 0$.

To ensure the condition for $|k| \geq R^{-1}$, we will use that $R < \delta d s \ell$ by Condition 1. We may then from the definitions (70) and (72) of τ_B assume that $\tau_B(k^2) \geq \frac{1}{2}k^2$ for $|k| \geq R^{-1} \geq \delta^{-1}(ds\ell)^{-1}$. For these k we thus have, since $|\mathcal{B}| = |B|^{-1}|\widehat{W}(k)| \leq Ca/|B|$, that

$$\mathcal{A} \geq \frac{1}{2}n^{-1}R^{-2} - Ca|B|^{-1} > Ca|B|^{-1}$$

if $n|B|^{-1} \leq c(aR^2)^{-1}$ for c sufficiently small (depending only on v_1). This implies that $\mathcal{A}$ is positive and that $\mathcal{A} \geq |\mathcal{B}|$.

In this case we are therefore allowed to use Theorem 4.5 to bound $h_\sigma(k)$ and in fact we may assume that $\mathcal{A}+\mathcal{B} \geq 2|\mathcal{B}|$ if c is sufficiently small. When the condition $n|B|^{-1} \leq c(aR^2)^{-1}$ can not be satisfied, which only happens on page 37 in Case 2 of the proof of Lemma 5.2, we use (64) instead.

4.6 LEMMA. *There exists $c > 0$ (depending only on v_1) such that if $n|B|^{-1} \leq c(aR^2)^{-1}$ then for all $k \in \mathbb{R}^3$*

$$h_\sigma(k) \geq -\left(n^{-1}\tau_B(k^2) + |B|^{-1}\widehat{W}(k) - \sqrt{n^{-2}\tau_B(k^2)^2 + 2n^{-1}|B|^{-1}\tau_B(k^2)\widehat{W}(k)}\right) n_0 \int \chi_B^2$$
$$- \sigma^2(n-\rho|B|)^2|B|^{-2}|\widehat{\chi}_B(k)|^2\widehat{W}(k) - C\sigma^2(n-\rho|B|)^2|B|^{-2}|\widehat{\chi}_B(k)|^2|\widehat{W}(k)|\mathbb{1}_{\{|k|\geq R^{-1}\}}(k), \tag{89}$$

where M is the integer in the definition (16) of χ.

Proof. As we just saw, we are in a situation where we can use Bogolubov's method from Theorem 4.5 with $\mathcal{A}+\mathcal{B} \geq 2|\mathcal{B}|$. This gives the estimate

$$2|\kappa|^2(\mathcal{A}+\mathcal{B})^{-1} \leq \sigma^2(n-\rho|B|)^2|B|^{-2}|\widehat{\chi}_B(k)|^2|\widehat{W}(k)|.$$

Now (89) follows, since we have already seen in (77) that $[b_k, b_k^*] \leq n_0 \int \chi_B^2$ and in (88) that $\widehat{W}(k) > 0$ for $|k| < R^{-1}$.

□

We shall primarily use the above lemma with $\sigma = 0$. On page 49 we will also use it with $\sigma = 1$ on the large box and then the second to last term in (89) will, after integration over k, give

$$-\frac{1}{2}(2\pi)^{-3}\sigma^2(n-\rho|B|)^2|B|^{-2}\int |\widehat{\chi}_B(k)|^2\widehat{W}(k)\,\mathrm{d}k = -\sigma^2(n-\rho|B|)^2\mathcal{U}_B,$$

using the notation (25), and hence exactly cancel the first positive term in (59). Recalling that $\chi_u(x) = \chi(x\ell^{-1} - u)$ and using (36) together with the estimate $|\widehat{W}(k)| \leq Ca$, we see that the last term in (89), after integration over k, will be bounded by

$$C\sigma^2|B|^{-1}a(n-\rho|B|)^2(R/\ell)^{2M}\int |k|^{2M}|\widehat{\chi}(k)|^2\,\mathrm{d}k \leq C\sigma^2|B|^{-1}a(n-\rho|B|)^2(R/\ell)^{2M}. \tag{90}$$

We have by Condition 1 that $R \ll \ell$ and this will be enough to control the last term in (89) if M is sufficiently large.

5 A Priori Bounds on the Non-Quadratic Part of the Hamiltonian and on n

We shall eventually prove that the lowest energy of the box Hamiltonian H_B will be achieved when the particle number n is close in an appropriate sense to $\rho|B|$. In this subsection we will give a much weaker a priori bound on n. The main difficulty lies in treating the (possibly) rectangular small boxes $B(u,u')$ of side lengths $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq d\ell$.

5.1 LEMMA (Estimates on the non-quadratic part of H_B)**.**
If B is a small box, we have

$$H_B - H_{\text{Quad}} \geq (1-\varepsilon_0)\varepsilon_T \widetilde{b}(d\ell)^{-2} n_+ + \left[\frac{7}{8}|n-\rho|B||^2 - C|n-\rho|B||n_+ - Cn - Cnn_+\right]\mathcal{U}_B \tag{91}$$

and if B is a large box, we have

$$H_B - H_{\text{Quad}} \geq (1-\varepsilon_0) b\ell^{-2} n_+ + \left[\frac{7}{8}|n-\rho|B||^2 - C|n-\rho|B||n_+ - Cn - Cnn_+\right]\mathcal{U}_B, \tag{92}$$

where $\widetilde{b}$ and b are the universal constants appearing in (42) *and* (49)*.*

Proof. We use estimate (59), Lemma 4.2 (with $\varepsilon_1' = \frac{|n-\rho B|}{8n}$), (64), (65), (66), (67), the respective Neumann gaps and the fact that $n_+ \leq n$ to obtain (91) and (92). □

The constant $\frac{7}{8}$ is of course not optimal and has been chosen for notational purposes only. To prove the next lemma, we would like to use that n_+ is much smaller than n. This follows from Lemma 4.1 in view of the following Condition, which we henceforth assume to hold.

CONDITION 3: *We require that*

$$(\sqrt{\rho a} d\ell)^2 \leq c_T \varepsilon_T, \tag{93}$$

where c_T is a small but universal constant.

5.2 LEMMA (A priori bound on n)**.**
There is a constant $C_0 > 0$ such that for any state with fixed particle number n on a small

box satisfying $\langle\psi|H_B|\psi\rangle \le 0$*, we have*

$$n \le C_0|B| \max\left\{\prod_{j=1}^{3}(\min\{\lambda_j, R\})^{-1}, \rho\right\}. \tag{94}$$

Proof. Assume $C_0 \ge 2$ and set

$$K_B = C_0|B| \max\left\{\prod_{j=1}^{3}(\min\{\lambda_j, R\})^{-1}, \rho\right\}.$$

Then $K_B \ge C_0|B|\prod_{j=1}^{3}\lambda_j^{-1} = C_0 \ge 2$. If $n \ge K_B$, let m be the integer part of nK_B^{-1}. We can then divide the particles into m groups of particles consisting of $n_1, \ldots, n_m$ particles where $\sum_{j=1}^{m} n_j = n$ and

$$\frac{1}{2}K_B \le n_j \le 2K_B, \quad j = 1, \ldots, m. \tag{95}$$

We now use that the interaction ω_B between the particles is non-negative and thereby get the following lower bound if we ignore the interactions between the groups and correct for the background self-energy term

$$\langle\psi|H_B|\psi\rangle - \rho^2|B|^2\mathcal{U}_B \ge m \inf\left\{\langle\psi'|H_B|\psi'\rangle - \rho^2|B|^2\mathcal{U}_B \middle| \psi' \text{ has } n' \text{ particles in } B,\ \frac{1}{2}K_B \le n' \le 2K_B\right\}.$$

Our aim is to prove that if C_0 is large enough, then

$$\langle\psi'|H_B|\psi'\rangle - \rho^2|B|^2\mathcal{U}_B \ge 0$$

if ψ' has particle number n' satisfying $K_B/2 \le n' \le 2K_B$. We have

$$\rho^2|B|^2 \le C_0^{-2}K_B^2 \le 4C_0^{-2}n'^2. \tag{96}$$

Using that $n' \ge \frac{C_0}{2}$, we have $n' \le \frac{2}{C_0}n'^2$ and $|n' - \rho|B|| \ge (1 - \frac{2}{C_0})n'$. With $n'_+ = \langle\psi' \mid n_+ \mid \psi'\rangle$ we obtain from Lemma 4.1, Lemma 5.1 and (96) that

$$\langle\psi'|H_B - H_{\text{Quad}}|\psi'\rangle - \rho^2|B|^2\mathcal{U}_B \ge (1 - \varepsilon_0)\varepsilon_T\widetilde{b}(d\ell)^{-2}n'_+ + \frac{3}{4}n'^2\mathcal{U}_B, \tag{97}$$

if C_0 is sufficiently large and δ sufficiently small. It remains to bound H_{Quad}. To do this, we differentiate between whether or not we are allowed to apply Bogolubov's method. With $c > 0$ being the constant in Lemma 4.6 which will allow us to use the Bogolubov bound, we first treat boxes where the side length and the parameter R are not too small in the sense that

Case I: $K_B < (c/2)|B|(aR^2)^{-1}$

Here we are allowed to use Bogolubov's method, i.e., Lemma 4.6. Combining (A.6), (A.7), (A.8) and (A.15), we get

$$\begin{aligned}\langle\psi'|H_{\mathrm{Quad}}|\psi'\rangle &\geq \frac{1}{2}(2\pi)^{-3}\int_{\mathbb{R}^3} h_0(k)\,\mathrm{d}k - Cn'_+ a\min\left\{R^{-3},|B|^{-1}\right\}\max\chi_B^2 \\ &\geq -Cn'a(ds\ell)^{-3}\max\chi_B^2 - Cn'\frac{n'}{|B|}a\frac{a}{R}\max\chi_B^2 - Cn'\frac{n'^2}{|B|^2}a^3R\max\chi_B^2 - Cn'\frac{a}{R^3}\max\chi_B^2 \\ &\geq -Cn'\frac{a}{R^3}\max\chi_B^2 - Cn'\frac{K_B}{|B|}a\frac{a}{R}\max\chi_B^2 - Cn'\frac{K_B^2}{|B|^2}a^3R\max\chi_B^2 \\ &\geq -Cn'\frac{a}{R^3}\max\chi_B^2. \end{aligned} \tag{98}$$

Using the lower bound in (27) together with (95) and (97), we have that

$$\begin{aligned}\langle\psi'|H_B|\psi'\rangle - \rho^2|B|^2\mathcal{U}_B &\geq Cn'^2\mathcal{U}_B - Cn'\frac{a}{R^3}\max\chi_B^2 \\ &= Cn'\mathcal{U}_B(n' - C\mathcal{U}_B^{-1}\frac{a}{R^3}\max\chi_B^2) \\ &\geq Cn'\mathcal{U}_B(n' - CC_0^{-1}n'),\end{aligned}$$

which is positive if C_0 is sufficiently large.

Case II: $K_B \geq (c/2)|B|(aR^2)^{-1}$

By Condition 1 and the Case II assumption we have

$$\frac{K_B}{|B|} = C_0\prod_{j=1}^{3}(\min\{\lambda_j,R\})^{-1} \geq \frac{c}{2}(aR^2)^{-1}. \tag{99}$$

Since $R,\lambda_j \leq d\ell$ we have $|B| \leq Ca(d\ell)^2$ such that $\max\chi_B^2 \leq C\left(\frac{a}{d\ell}\right)^{4(M+1)}$ by (19). By Lemma 4.1 and Condition 3, we have $n_+ \leq Cc_T n\max\chi_B^2$. From the lower bound in (27) we get

$$\begin{aligned}Cn'^2_+\frac{a}{R^3}\max\chi_B^2 &\leq Cc_Tn'^2\frac{a}{R^3}\max\chi_B^4 \\ &\leq Cc_Tn'^2|B|\prod_{j=1}^{3}(\min\{\lambda_j,R\})^{-1}\max\chi_B^2\,\mathcal{U}_B \\ &\leq Cc_Tn'^2\left(\frac{d\ell}{R}\right)^3\left(\frac{a}{d\ell}\right)^{4(M+1)}\mathcal{U}_B.\end{aligned}$$

Together with equation (97) and the estimate

$$\langle \psi' | H_{\text{Quad}} | \psi' \rangle \geq \langle \psi' | \mathcal{Q}_2' | \psi' \rangle \geq -\frac{5}{8} n'^2 \mathcal{U}_B - C n_+^2 \frac{a}{R^3} \max \chi_B^2,$$

which follows from (64), this yields

$$\langle \psi' | H_B | \psi' \rangle - \rho^2 |B|^2 \mathcal{U}_B \geq \frac{1}{8} n'^2 \mathcal{U}_B - C n_+'^2 a R^{-3} \max \chi_B^2 \geq 0,$$

provided δ is sufficiently small. □

When applying the above lemma, we will assume that the box $B = B(u, u')$ has either smallest side length $\lambda_1 \leq \rho^{-\frac{1}{3}}$ or $\lambda_1 > \rho^{-\frac{1}{3}}$. Note that if $\lambda_1 > \rho^{-\frac{1}{3}}$, we get $n \leq C_0 |B| \max \{R^{-3}, \rho\}$ and may apply Lemma 4.6.

5.1 A Priori Bounds on the Energy in the Small Box

Small boxes at the boundary of the large box may be arbitrarily small. We first consider the case of boxes which are so small that Bogolubov's method can not be applied. By the lemma below these boxes only contribute to $e_0(\rho)$ by an amount, which is of lower order than the LHY-term.

5.3 LEMMA (Lower bound on the energy on small boxes with $\lambda_1 \leq \rho^{-\frac{1}{3}}$).
Let $B = B(u,u')$ be a small box with smallest side length $\lambda_1 \leq \rho^{-\frac{1}{3}}$. Then

$$\langle H_B \rangle \geq -C|B| \max\left\{\rho, R^{-3}\right\} \frac{a}{R^3} \left(\frac{\rho^{-\frac{1}{3}}}{d\ell}\right)^{4M+2}, \tag{100}$$

where M is the integer in the definition (16) of χ. For all $u \in \mathbb{R}^3$

$$\int_{\lambda_1(B(u,u')) \leq \rho^{-\frac{1}{3}}} H_{uu'} \, \mathrm{d}u' \geq -C\mathcal{L}, \tag{101}$$

with $\mathcal{L} = |B| \max\left\{\rho, R^{-3}\right\} \frac{a}{R^3} \left(\frac{\rho^{-\frac{1}{3}}}{\ell}\right)^{2M}$.

Proof. We use Lemma 4.1 to get the bound $\langle H_B \rangle \geq -Cn\rho|B|\mathcal{U}_B$. Since we may assume that $\langle H_B \rangle \leq 0$, we use Lemma 5.2, which together with $\lambda_1 \leq \rho^{-\frac{1}{3}}$ gives $n \leq C|B| \prod_{j=1}^{3} \min\left\{\lambda_j, R\right\}^{-1}$. Using the upper bound in (27) followed by (19), we arrive at

$$\begin{aligned}\langle H_B \rangle \geq & - C \frac{|B|^2}{\prod_{j=1}^{3} \min\left\{\lambda_j, R\right\}} \rho \frac{a}{R^3} \max \chi_B^2 \\ \geq & - C \frac{\lambda_1 (d\ell)^2 |B|}{\min\left\{\lambda_1^3, R^3\right\}} \rho \frac{a}{R^3} \left(\frac{\lambda_1}{\ell}\right)^{2(M+1)}.\end{aligned} \tag{102}$$

The estimate in (101) is obtained by integrating over u' such that $B(u,u')$ has $\lambda_1 \leq \rho^{-\frac{1}{3}}$, which gives a volume smaller than $Cd^{-2}\frac{\rho^{-\frac{1}{3}}}{d\ell}$, and using that $\lambda_1 \leq \rho^{-\frac{1}{3}} < d\ell$. □

Now we turn to the case of small boxes which have smallest side length larger than $\rho^{-\frac{1}{3}}$ and where Bogolubov's method (Lemma 4.6) therefore is applicable.

5.4 LEMMA (2^{nd} a priori bound on n for small boxes with $\lambda_1 \geq \rho^{-\frac{1}{3}}$).
If B is a small box with $\lambda_1 \geq \rho^{-\frac{1}{3}}$, then there exists a constant $C_1 > 1$ such that for any state of fixed particle number n satisfying $\langle \psi | H_B | \psi \rangle \leq 0$ we have

$$n \leq C_1 \rho |B|.$$

Proof. We may assume that $R \leq \rho^{-\frac{1}{3}}$, since otherwise the lemma follows from the first a priori bound on n in Lemma 5.2. Hence the estimates (27) and (28) give

$$C^{-1}\frac{a}{|B|}\max\chi_B^2 \leq \mathcal{U}_B \leq C\frac{a}{|B|}\max\chi_B^2. \tag{103}$$

Assume $n \geq C_1\rho|B|$ with $C_1 > 1$. Note here that $\rho|B| \geq \rho\rho^{-1} = 1$ since $\lambda_1 \geq \rho^{-\frac{1}{3}}$ and we therefore actually have that $n \geq C_1$. Using Lemma 4.1, we see from Lemma 4.4, Lemma 5.1 and (103) that

$$\begin{aligned} H_B &\geq Cn^2\frac{a}{|B|}\max\chi_B^2 + \frac{1}{2}(2\pi)^{-3}\int h_0(k)\,\mathrm{d}k - Cn_+\frac{a}{|B|}\max\chi_B^2 \\ &\geq Cn^2\frac{a}{|B|}\max\chi_B^2 + \frac{1}{2}(2\pi)^{-3}\int h_0(k)\,\mathrm{d}k, \end{aligned} \tag{104}$$

provided C_1 is sufficiently large and δ is sufficiently small. Combining (A.6), (A.7), (A.8) and (A.15) in the appendix, we get

$$\int h_0(k)\,\mathrm{d}k \geq -C\frac{n}{|B|}(ds\ell)^{-3}\int\chi_B^2 - C\frac{n^2}{|B|^2}\frac{a^2}{R}\int\chi_B^2 - C\frac{n^3a^3}{|B|^3}R\int\chi_B^2. \tag{105}$$

Now we use the assumption $n \geq C_1\rho|B|$ and that $n \leq C_0|B|R^{-3}$ by Lemma 5.2

$$0 \geq H_B \geq \left(Cn^2 - Cn^2\rho^{-1}(ds\ell)^{-3} - Cn^2\frac{a}{R} - Cn^2\frac{a^2}{R^2}\right)\frac{a}{|B|}\max\chi_B^2.$$

By Condition 1 we have $C - C(\frac{\rho^{-\frac{1}{3}}}{ds\ell})^3 - C\frac{a}{R} - C\frac{a^2}{R^2} > 0$, if δ is sufficiently small, which is a contradiction.

□

5.5 LEMMA (Lower bound on the energy on small boxes with $\lambda_1 > \rho^{-\frac{1}{3}}$).
If B is a small box with $\lambda_1 \geq \rho^{-\frac{1}{3}}$ and ψ is a state with fixed particle number n satisfying $\langle\psi|H_B|\psi\rangle \leq 0$, then

$$\begin{aligned} \langle H_B\rangle \geq\ & C\varepsilon_T\widetilde{b}(d\ell)^{-2}n_+ + \frac{3}{4}|n-\rho|B||^2\mathcal{U}_B - C\rho a \\ & - \frac{1}{4}(2\pi)^{-3}\frac{1}{R}\rho^2\int\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k\int\chi_B^2 - C\rho^2a(\rho a^3)^{\frac{1}{2}}\mathcal{S}_1\int\chi_B^2, \end{aligned}$$

where

$$\mathcal{S}_1 = \varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R} + (\sqrt{\rho a}ds\ell)^{-1}\ln\left(\frac{ds\ell}{R}\right) + \sqrt{\rho a}R + (\sqrt{\rho a}ds\ell)^{-3} + (\rho a^3)^{-\frac{1}{2}}\frac{a^2}{R^2}\max\{\rho R^3, 1\}. \tag{106}$$

Proof. We estimate the non-quadratic part of H_B using Lemma 5.1 together with Lemma 5.4, yielding $n \leq C\rho|B|$. Since $\mathcal{U}_B \leq C\frac{a}{|B|}$ by (28), this gives terms of the form $C\rho a n_+$, but these can be absorbed into the Neumann gap since $(d\ell\sqrt{\rho a})^2 < c_T\varepsilon_T$ by Condition 3. Hence we obtain

$$H_B - H_{\text{Quad}} \geq C\varepsilon_T\widetilde{b}(d\ell)^{-2}n_+ + \frac{7}{8}|n - \rho|B||^2\mathcal{U}_B - C\rho a. \tag{107}$$

We use Lemma 4.4 with $\sigma = 0$ to estimate the quadratic part

$$H_{\text{Quad}} \geq \frac{1}{2}(2\pi)^{-3}\int_{\mathbb{R}^3} h_0(k)\,\mathrm{d}k - Cn_+a\min\{R^{-3}, |B|^{-1}\}\max\chi_B^2. \tag{108}$$

Using the bounds (A.4), (A.6), (A.8) and (A.15) in the appendix, we obtain

$$\begin{aligned}\frac{1}{2}(2\pi)^{-3}\int h_0(k)\,\mathrm{d}k \geq& -\frac{1}{4}(2\pi)^{-3}(1+C\varepsilon_0)\frac{1}{R}\int\left(\frac{n}{|B|}\right)^2\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k\int\chi_B^2 \\ &- C\rho^2 a\frac{a}{ds\ell}\ln\left(\frac{ds\ell}{R}\right)\int\chi_B^2 - C(\rho a)^3 R\int\chi_B^2 \\ &- C\rho a(ds\ell)^{-3}\int\chi_B^2.\end{aligned} \tag{109}$$

The second term in (108) is smaller than $Cn_+\rho a$, since we assumed that $\lambda_1 \geq \rho^{-\frac{1}{3}}$, and may therefore also be absorbed into the Neumann gap. Instead of estimating the term $|n - \rho|B||$, we can use that if $C_1 > 0$, then

$$-\frac{1}{4}(2\pi)^{-3}\left(\frac{n}{|B|}\right)^2\frac{1}{R}\int\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k\int\chi_B^2 + C_1|n-\rho|B||^2\mathcal{U}_B \tag{110}$$

$$\geq -\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k\int\chi_B^2 - C\rho^2 a\frac{a^2}{R^2}\max\{\rho R^3, 1\}\int\chi_B^2. \tag{111}$$

To see that this is possible, we note that by (27)

$$\mathcal{U}_B \geq C\min\left\{\frac{\rho^{-1}}{R^2}, R\right\}\frac{1}{R}\frac{a}{|B|}\max\chi_B^2.$$

The n^2-term in (110) is therefore positive if δ is sufficiently small and we can verify (111) by optimizing over n and noticing that the optimal particle number satisfies $n \leq \rho|B|(1 + C\frac{a}{R}\max\{\rho R^3, 1\})$. $\square$

6 Estimates on the Large Box

From now on we will only focus on the large box, where we have $\int \chi_B^2 = |B|$. The following lemma gives a lower bound for the operator H_B on the large box and is the starting point for the bounds on n_+ and $|n - \rho|B||$ on the large box.

6.1 LEMMA. *On a large box we have*

$$
\begin{aligned}
H_B \geq & -\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| \\
& + Cb\ell^{-2}n_+ - C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_2,
\end{aligned} \tag{112}
$$

where

$$
\begin{aligned}
\mathcal{S}_2 = & (\sqrt{\rho a}ds\ell)^{-3} + \varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R} + \sqrt{\rho a}R + (\sqrt{\rho a}ds\ell)^{-1}\ln\left(\frac{ds\ell}{R}\right) \\
& + (\rho a^3)^{-\frac{1}{2}}\frac{a^2}{R^2}\max\{\rho R^3, 1\} + (\sqrt{\rho a}d\ell)^{-3} + \left(\rho^2 a|B|\sqrt{\rho a^3}\right)^{-1}\mathcal{L},
\end{aligned} \tag{113}
$$

such that $\mathcal{S}_2 = \mathcal{S}_1 + (\sqrt{\rho a}d\ell)^{-3} + \left(\rho^2 a|B|\sqrt{\rho a^3}\right)^{-1}\mathcal{L}$. *Here* $\mathcal{L}$ *is the contribution from the small boxes with* $\lambda_1 \leq \rho^{-\frac{1}{3}}$ *in* (101).

Proof. We use Lemma 3.10, together with (18), and sum the contribution of the small boxes. We use Lemma 5.5 for boxes with $\lambda_1 > \rho^{-\frac{1}{3}}$, of which we have less then Cd^{-3}. For the small boxes boxes with $\lambda_1 \leq \rho^{-\frac{1}{3}}$ we use Lemma 5.3. □

In the end of this section we will choose our parameters such that the first term in (113) is the largest, allowing us to write $\mathcal{S}_2 = (\sqrt{\rho a}ds\ell)^{-3}$.

6.2 LEMMA (Control of $\langle n_+\rangle$ in the large box)**.**
For any state on the large box, which satisfies

$$
\langle H_B\rangle \leq -\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| + C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_2, \tag{114}
$$

we have

$$
\langle n_+\rangle \leq C\rho|B|\sqrt{\rho a^3}\mathcal{S}_3, \tag{115}
$$

where $\mathcal{S}_3 = \rho a\ell^2\mathcal{S}_2$ *and* $\mathcal{S}_2$ *is given by* (113).

Proof. Simply apply Lemma 6.1. □

The parameters $\mathcal{S}_1, \mathcal{S}_2$ and $\mathcal{S}_3$ essentially originate from the a priori estimate on the small box. By Condition 1 we have that $1 \ll \mathcal{S}_1 \ll \mathcal{S}_2 \ll \mathcal{S}_3$. The exact form of $\mathcal{S}_2$, and hence $\mathcal{S}_3$, is not important. With our choice of parameters and Condition 4 below we have that $\mathcal{S}_2 \leq C(\sqrt{\rho a} ds\ell)^{-3}$, which asymptotically is slightly larger than 1. Note that Condition 4 ensures that the second term in (114), while being larger than the LHY-order, is of lower order than the leading order term. We therefore have that $\langle H_B \rangle \leq 0$ if the requirement in Lemma 6.2 is satisfied and δ is sufficiently small. In this section we will introduce new error terms and these will be smaller than the LHY-order.

CONDITION 4: *We require*

$$\sqrt{\rho a^3}\mathcal{S}_3 < \delta \frac{a}{R}.$$

6.3 LEMMA. *If B is a large box and a state with fixed particle number satisfies*

$$\langle H_B \rangle \leq -\frac{1}{4}(2\pi)^{-3}\rho^2 \frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| + C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_2,$$

then $n \leq C\rho|B|$ and

$$\langle H_{\text{Quad}} \rangle \geq -\frac{1}{4}(2\pi)^{-3}\left(\frac{n}{|B|}\right)^2 \frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| - C\mathcal{E}_{\text{Quad}}\rho^2 a\sqrt{\rho a^3}|B|, \tag{116}$$

where

$$\begin{aligned}\mathcal{E}_{\text{Quad}} = {} & (\sqrt{\rho a}s\ell)^{-3} + (\rho a^3)^{\frac{1}{2}}\frac{R}{a} + \varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R} \\ & + (\sqrt{\rho a}s\ell)^{-1}\ln\left(\frac{s\ell}{R}\right) + \varepsilon_T(\sqrt{\rho a}ds\ell)^{-1}\ln\left(\frac{ds\ell}{R}\right).\end{aligned}$$

Proof. We start with the bound on n. From Lemma 4.4, (A.2) and (A.16) we obtain

$$H_{\text{Quad}} \geq -C(s\ell)^{-3}\frac{a}{|B|}n|B| - Cn^2\frac{a}{R}\frac{a}{|B|} - Cn_+\frac{a}{|B|}.$$

Note that $n_+ \leq C(\rho a^3)^{\frac{1}{2}}\mathcal{S}_3 n < C\delta\frac{a}{R}n$ by Lemma 6.2 and that $\langle H_B \rangle \leq 0$ by Condition 4 if δ is sufficiently small. Assume that $n \geq C\rho|B|$. It then follows from Lemma 5.1 that $\langle H_B - H_{\text{Quad}} \rangle \geq Cn^2\frac{a}{|B|}$ if δ is sufficiently small and we obtain the contradiction

$$0 \geq \langle H_B \rangle \geq \left(Cn^2 - Cn^2(s\ell)^{-3}\rho^{-1} - Cn^2\frac{a}{R} - Cn^2 aR^{-2}\right)\frac{a}{|B|}.$$

Hence $n \leq C\rho|B|$. Now we use (A.4) together with (A.16), (A.18) and (A.22) to obtain a lower bound on $\langle H_{\mathrm{Quad}}\rangle$. □

The important difference to the estimate on the small box is that $\mathcal{E}_{\mathrm{Quad}} \ll 1$ by Condition 4.

6.4 LEMMA (Improved bound on n on the large box)**.**
If B is a large box and a state satisfies

$$\langle H_B\rangle \leq -\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| + C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_2,$$

then

$$|n-\rho|B|| \leq C\rho|B|\left(\rho a^3\right)^{\frac{1}{4}}\mathcal{S}_3{}^{\frac{1}{2}}. \tag{117}$$

Proof. We use the bound on the non-quadratic part in Lemma 5.1, the bound on H_{Quad} in Lemma 6.3, the bound on n_+ in Lemma 6.2 and, analogously to (111), a part of the positive term $|n-\rho|B||$ to control the integral corresponding to the second Born term and obtain

$$\begin{aligned}\langle H_B\rangle \geq{}& C\ell^{-2}n_+ + \left[\frac{7}{8}|n-\rho|B||^2 - C|n-\rho|B||n_+ - Cn - Cnn_+\right]\mathcal{U}_B\\ &-\frac{1}{4}(2\pi)^{-3}\left(\frac{n}{|B|}\right)^2\frac{1}{R}\int\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| - C\rho^2 a\sqrt{\rho a^3}|B|\mathcal{E}_{\mathrm{Quad}}\\ \geq{}& \left[C|n-\rho|B||^2 - C\rho^2|B|^2\sqrt{\rho a^3}\mathcal{S}_3\right]\frac{a}{|B|}\\ &-\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int\frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| - C\rho^2 a\sqrt{\rho a^3}|B|\mathcal{E}_{\mathrm{Quad}} - C\rho^2 a\frac{a^2}{R^2}|B|.\end{aligned}$$

Hence $|n-\rho|B|| \leq C\rho|B|\left(\rho a^3\right)^{\frac{1}{4}}\mathcal{S}_3{}^{\frac{1}{2}}$, by Condition 1. □

We will apply the following theorem, whose proof can be found in [13].

6.5 THEOREM (Localization of large matrices)**.**
Suppose that $\mathcal{A}$ is an $(N+1)\times(N+1)$ Hermitean matrix and let $\mathcal{A}^k$, with $k=0,1,\ldots,N$, denote the matrix consisting of the k^{th} supra- and infra-diagonal of $\mathcal{A}$. Let $\psi\in\mathbb{C}^{N+1}$ be a normalized vector and set $d_k=\langle\psi,\mathcal{A}^k\psi\rangle$ and $\lambda=\langle\psi,\mathcal{A}\psi\rangle=\sum_{k=0}^{N}d_k$ (ψ need not be an eigenvector of $\mathcal{A}$). Choose some positive integer $\mathcal{M}\leq N+1$. Then, with $\mathcal{M}$ fixed, there is some $n\in[0,N+1-\mathcal{M}]$ and some normalized vector $\phi\in\mathbb{C}^{N+1}$ with the property that

$\phi_j = 0$ unless $n+1 \le j \le n+\mathcal{M}$ (i.e., ϕ has length $\mathcal{M}$) and such that

$$\langle \phi, \mathcal{A}\phi\rangle \le \lambda + \frac{C}{\mathcal{M}^2}\sum_{k=1}^{\mathcal{M}-1} k^2|d_k| + C\sum_{k=\mathcal{M}}^{N}|d_k|, \tag{118}$$

where $C>0$ is a universal constant. (Note that the first sum starts at $k=1$.)

We apply the theorem in the following way. Let Ψ be a (normalized) n-particle wave function. Since the n-particle sector of Fock space is spanned by n_+-eigenfunctions, we can write $\Psi = \sum_{m=0}^{n} c_m\Psi_m$, with Ψ_m normalised and $n_+\Psi_m = m\Psi_m$ for $m \in \{0,1,\dots,n\}$. This lets us consider the $(n+1)\times(n+1)$ Hermitean matrix $\mathcal{A}_{m,m'} = \langle \Psi_m, H_B\Psi_{m'}\rangle$ and the vector $\psi = (c_0, c_1, \dots, c_n)$. From the form of H_B we obtain that $d_k = 0$ for $k \ge 3$. In Section 6.1 we will show that $|d_1| + |d_2| \le C\rho^2 a|B|\frac{a}{R}$. We may assume that

$$\begin{aligned}\langle \Psi, H_B\Psi\rangle \le &-\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| \\ &+ 4\pi\rho^2 a|B|\sqrt{\rho a^3}\frac{128}{15\sqrt{\pi}}.\end{aligned} \tag{119}$$

From Theorem 6.5 we obtain a (normalized) state, $\widetilde{\psi}$, which has n_+-eigenvalues localized to an interval of length $\mathcal{M}$ and an energy that satisfies the bound

$$\langle \widetilde{\psi}, H_B\widetilde{\psi}\rangle - C\mathcal{M}^{-2}\left(|d_1| + |d_2|\right) \le \langle \Psi, H_B\Psi\rangle. \tag{120}$$

We will spend the rest of this section on establishing a lower bound for $\langle \widetilde{\psi}, H_B\widetilde{\psi}\rangle$. For this purpose we introduce the following condition on $\mathcal{M}$. Note that (120) also holds if we add $-\varepsilon_0\Delta_u^{\mathcal{N}}$ on both sides.

CONDITION 5: *We require*

(i) $\frac{a}{R}\mathcal{M}^{-2} < C\sqrt{\rho a^3}\mathcal{S}_2$

(ii) $\rho|B|\sqrt{\rho a^3}\mathcal{S}_3 = (\sqrt{\rho a}\ell)^3\mathcal{S}_3 \le \mathcal{M}$.

From (120) and Conditions 1 and 5 it follows that

$$\langle \widetilde{\psi}, H_B\widetilde{\psi}\rangle \le -\frac{1}{4}(2\pi)^{-3}\rho^2\frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k|B| + C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_2. \tag{121}$$

Hence Lemmas 6.2, 6.3 and 6.4 apply to $\widetilde{\psi}$. We obtain from Lemma 6.2 and Condition 5 that $n_+ \le C_0\mathcal{M}$. This gives the estimate $\langle n_+^m\rangle \le C_0^{m-1}\langle n_+\rangle\mathcal{M}^{m-1}$ for the state $\widetilde{\psi}$. In particular, we obtain

$$\langle\widetilde{\psi}|n_+^2|\widetilde{\psi}\rangle \leq C\mathcal{M}\langle\widetilde{\psi}|n_+|\widetilde{\psi}\rangle, \tag{122}$$

which we will use to ensure that Lemma 6.6 may be used for the state $\widetilde{\psi}$.

6.1 Control of d_1 and d_2.

In this subsection we show that $|d_1| + |d_2| \leq C\rho^2 a|B|\frac{a}{R}$. By definition d_1 is the expectation in the state Ψ of the terms with 1-Q and 3-Q. From Lemma 4.2, equation (66), which could have been stated as two-sided bounds, and that $n \leq C\rho|B|$, we obtain by setting $\varepsilon_1' = c\frac{|n-\rho|B||}{\rho|B|}$ with c sufficiently small and $\varepsilon_1'' = 1$

$$\begin{aligned}|d_1| &= |\langle\Psi, (\mathcal{Q}_1' + \mathcal{Q}_1'' + \mathcal{Q}_3)\,\Psi\rangle| \\ &\leq (n-\rho|B|)^2\,\frac{a}{|B|} + C\langle\Psi|\rho a((1+\varepsilon_3^{-1})n_+ + 1)|\Psi\rangle + \varepsilon_3\langle\Psi|\sum_{i<j}Q_jQ_iw_B(x_i,x_j)Q_iQ_j|\Psi\rangle.\end{aligned}$$

We can use Lemmas 6.2 and 6.4 together with Conditions 1 and 4 to see that

$$(n-\rho|B|)^2\,\frac{a}{|B|} + C\langle\Psi|\rho a((1+\varepsilon_3^{-1})n_+ + 1)|\Psi\rangle \leq C\rho^2|B|a\frac{a}{R},$$

as long as we choose ε_3 to be a constant. However, we can not easily bound

$$\langle\Psi|\sum_{i<j}Q_jQ_iw_B(x_i,x_j)Q_iQ_j|\Psi\rangle.$$

We may assume that

$$\langle\Psi|\sum_{i<j}Q_jQ_iw_B(x_i,x_j)Q_iQ_j|\Psi\rangle \leq C\rho^2 a|B|\frac{a}{R},$$

since otherwise we get using Condition 4

$$\langle\Psi|H_B - H_{\mathrm{Quad}}|\Psi\rangle \geq C|n-\rho|B||^2\frac{a}{|B|} + C\rho^2 a|B|\frac{a}{R}, \tag{123}$$

which would contradict (119) in view of Lemma 6.3. It follows that $|d_1| \leq C\rho^2 a|B|\frac{a}{R}$.

We now estimate d_2, which with our notation corresponds to the second sum in the definition of $\mathcal{Q}_2'$ on page 27, respectively the terms containing b^*b^* and bb appearing in H_{Quad}. We bound $|d_2|$ using equation (86) with $\mathcal{A}$ and $\mathcal{B}$ as in (87). From Theorem 6.3 we know that

$$\langle\Psi|\frac{1}{2}(2\pi)^{-3}\left(n^{-1}\tau_B(k^2)+|B|^{-1}\widehat{W}(k)-\sqrt{n^{-2}\tau_B(k^2)+2n^{-1}|B|^{-1}\tau_B(k^2)\widehat{W}(k)}\right)n_0\int\chi_B^2|\Psi\rangle$$
$$\leq C\rho^2 a|B|\frac{a}{R}.$$

It is therefore left to show that

$$\langle\Psi|\frac{1}{2}(2\pi)^{-3}n^{-1}\int\tau_B(k^2)b_k^*b_k\,\mathrm{d}k|\Psi\rangle\leq C\rho^2 a|B|\frac{a}{R} \tag{124}$$

and that

$$|B|^{-1}\langle\Psi|\frac{1}{2}(2\pi)^{-3}\int\widehat{W}_B(k)b_k^*b_k\,\mathrm{d}k|\Psi\rangle\leq C\rho^2 a|B|\frac{a}{R}. \tag{125}$$

We show (125) first. As on page 30 we may assume that $n_+\geq 1$. From (82) and Lemma 4.3 we then see that

$$\begin{aligned}|B|^{-1}\langle\Psi|\int\widehat{W}_B(k)b_k^*b_k\,\mathrm{d}k|\Psi\rangle&=|B|^{-1}\langle\Psi|\int\widehat{W}_B(k)a(Q(\chi_B e^{ikx}))^*na(Q(\chi_B e^{ikx}))\,\mathrm{d}k|\Psi\rangle\\&\leq C|B|^{-1}a\langle\Psi|nn_+|\Psi\rangle\\&\leq C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_3\\&\leq C\rho^2 a|B|\frac{a}{R},\end{aligned}$$

where we also used Lemma 6.2, that $n\leq C\rho|B|$ and Condition 4.

We now show (124). Repeating the estimate for the lower bound on H_{Quad} with only half of the term in (124) included would again give a lower bound of order $\rho^2|B|a\frac{a}{R}$ because the second Born approximation to a would be calculated wrong to this order. If (124) would not hold this would give that $\langle\Psi|H_{\mathrm{Quad}}|\Psi\rangle\geq 0$, which contradicts the assumption in (119). Hence we arrive, as stated on page 45, at the estimate

$$|d_1|+|d_2|\leq C\rho^2 a|B|\frac{a}{R}. \tag{126}$$

The following lemma will be used to control the expectation of the second term in $\mathcal{Q}_3$, see (66), in the state $\widetilde{\psi}$ when $\varepsilon_3 \gg 1$.

6.6 LEMMA. *With*

$$h := \sum_{i=1} -\varepsilon_0 \Delta^{\mathcal{N}}_{u,i} - \varepsilon_3 \sum_{i<j} Q_j Q_i w_B(x_i, x_j) Q_i Q_j \tag{127}$$

we have

$$\langle \psi, h\psi \rangle \geq 0, \tag{128}$$

provided $\varepsilon_0 \langle \psi, n_+ \psi \rangle \geq C_0 \varepsilon_3 \frac{a}{R} \langle \psi, n_+^2 \psi \rangle$ *with* C_0 *sufficiently large and depending only on* v_1*.*

Proof. The operator h acts in Fock space and commutes with n_+. In fact, h only depends on the excited particles in the following sense. We can identify the Fock space as $\mathcal{F}(L^2(B)) = \mathcal{F}(QL^2(B)) \otimes \mathcal{F}(PL^2(B))$. In this representation h is an operator acting only on the first factor. In a fixed n_+ subspace of this factor the operator has the form

$$h = \sum_{i=1}^{n_+} \big(-\varepsilon_0 \Delta^{\mathcal{N}}_i - \varepsilon_3 \sum_{j=i+1}^{n_+} Q_i Q_j w_B(x_i, x_j) Q_i Q_j \big).$$

If ψ is in this subspace, we have

$$\langle \psi, h\psi \rangle = \sum_{i=1}^{n_+} \Big(\langle \psi, -\varepsilon_0 \Delta^{\mathcal{N}}_i \psi \rangle - \varepsilon_3 \sum_{j=i+1}^{n_+} \langle \psi, w_B(x_i, x_j) \psi \rangle \Big).$$

Note that a function ϕ, orthogonal to constants, i.e., $\phi \in QL^2(B)$ satisfies the Sobolev inequality $\langle \phi, -\Delta^{\mathcal{N}} \phi \rangle \geq C \|\phi\|_6^2$. This implies that if ψ is normalized, then

$$\begin{aligned}
&\sum_{i=1}^{n_+} \int \varepsilon_0 |\nabla_i \psi(x_1, \ldots, x_{n_+})|^2 - \varepsilon_3 \sum_{j=i+1}^{n_+} \omega_B(x_i, x_j) |\psi(x_1, \ldots, x_{n_+})|^2 \, \mathrm{d}x_1 \cdots \mathrm{d}x_{n_+} \\
&= n_+ \int \varepsilon_0 |\nabla_1 \psi(x_1, \ldots, x_{n_+})|^2 - \varepsilon_3 \tfrac{(n_+ - 1)}{2} \omega_B(x_1, x_2) |\psi(x_1, \ldots, x_{n_+})|^2 \, \mathrm{d}x_1 \cdots \mathrm{d}x_{n_+} \\
&\geq \int \Big(C\varepsilon_0 n_+ - \varepsilon_3 \tfrac{n_+^2}{2} ||\omega_B(\,\cdot\,, x_2)||_{\frac{3}{2}} \Big) \Big(\int |\psi(x_1, \ldots, x_{n_+})|^6 \, \mathrm{d}x_1 \Big)^{\frac{1}{3}} \mathrm{d}x_2 \cdots \mathrm{d}x_{n_+} \\
&\geq \Big(C\varepsilon_0 n_+ - C\varepsilon_3 n_+^2 \frac{a}{R} \Big) \int \Big(\int |\psi(x_1, \ldots, x_{n_+})|^6 \, \mathrm{d}x_1 \Big)^{\frac{1}{3}} \mathrm{d}x_2 \cdots \mathrm{d}x_{n_+} \\
&\geq 0,
\end{aligned}$$

where we have used that $\int \omega_B(x,y)^{\frac{3}{2}}\,\mathrm{d}x \leq C\int W(x-y)^{\frac{3}{2}}\,\mathrm{d}x \leq C\int v_R(x)^{\frac{3}{2}}\,\mathrm{d}x \leq C\left(\frac{a}{R}\right)^{\frac{3}{2}}$. □

6.2 Obtaining the LHY-Constant with Error Terms

CONDITION 6: *We require*

$$\varepsilon_0 > C\varepsilon_3 \frac{a}{R}\mathcal{M}.$$

From (122) and Condition 6 we obtain that the requirement in Lemma 6.6 is satisfied for the state $\widetilde{\psi}$. As mentioned on page 28, we can not absorb the second term in (66) into the positive term $\langle\widetilde{\psi}, \mathcal{Q}_4\widetilde{\psi}\rangle$ if $\varepsilon_3 > 1$, but we can use the kinetic energy $-\varepsilon_0\Delta_u^{\mathcal{N}}$ that we have saved in Theorem 3.10. Applying Lemmas 6.2, 6.3 and 6.6, we obtain the lower bound

$$\langle\widetilde{\psi}, \left(-C\varepsilon_3^{-1}nn_+\mathcal{U}_B - \varepsilon_0\Delta_u^{\mathcal{N}} - \varepsilon_3 QQw_B(x,y)QQ\right)\widetilde{\psi}\rangle \geq -C\rho^2 a|B|(\rho a^3)^{\frac{1}{2}}\mathcal{S}_3\varepsilon_3^{-1}, \tag{129}$$

where $-\varepsilon_0\Delta_u^{\mathcal{N}}$ is the kinetic energy that we have saved in Theorem 3.10.

The estimates on n_+ and $|n-\rho|B||$ in Lemma 6.2 and 6.4 do not give sufficiently good bounds on $\langle\widetilde{\psi}|\mathcal{Q}_1'|\widetilde{\psi}\rangle$. This problem is resolved by estimating $\mathcal{Q}_1'$ together with H_{Quad}, i.e., using Lemma 4.4 with $\sigma = 1$ instead of $\sigma = 0$. As already explained on page 33, this gives the additional term $-|n-\rho|B||^2\mathcal{U}_B$, which exactly cancels the first term in $\mathcal{Q}_0$, and an additional term, which is much smaller than the LHY-order. Choosing $\varepsilon_1'' = (\rho|B|)^{-\frac{1}{2}}\mathcal{M}^{\frac{1}{2}}$ we have

$$\begin{aligned}
&\langle\widetilde{\psi}|(\mathcal{Q}_0 - |n-\rho|B||^2) + \mathcal{Q}_1'' + \mathcal{Q}_2''|\widetilde{\psi}\rangle \\
\geq &-\langle\widetilde{\psi}|\left[-C|n-\rho|B||n_+ + n_+^2 - n_0 - \varepsilon_1''(n_+ + 1)n_0 - C\varepsilon_1''^{-1}n_+^2 - Cn_+^2\right]\mathcal{U}_B|\widetilde{\psi}\rangle \\
\geq &-C\rho^2 a|B|\sqrt{\rho a^3}(\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{3}{2}} - C\rho^2 a|B|\sqrt{\rho a^3}\mathcal{S}_3(\rho|B|)^{-\frac{1}{2}}\mathcal{M}^{\frac{1}{2}}.
\end{aligned} \tag{130}$$

It is left to estimate the integral appearing in $\langle\widetilde{\psi}|H_{\text{Quad}} + \mathcal{Q}_1'|\widetilde{\psi}\rangle|B|^{-1}$.

The value $4\pi\frac{128}{15\sqrt{\pi}}$ for the LHY-term is obtained by integrating over values of k close to $\sqrt{\rho a}$ after essentially subtracting a part of the second Born term. For the following estimate we note that $\int \chi_B^2 = |B|$ on the large box and that for a lower bound n_0 may be replaced by n in the expression for h_0 since $h_0 \leq 0$ as explained in (A.5) in the Appendix.

$$\frac{1}{2}(2\pi)^{-3}\int_{(s\ell)^{-1}<|k|<R^{-1}} h_0(k) + \frac{1}{2}\frac{n^2\widehat{W}(k)^2}{|B|\tau_B(k^2)}\,\mathrm{d}k|B|^{-1} \tag{131}$$

$$\geq \frac{1}{2}(2\pi)^{-3}\int_{(s\ell)^{-1}<|k|<R^{-1}} \tau_B(k^2)\left(\sqrt{1+2\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}}-1-\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}+\frac{1}{2}\frac{n^2\widehat{W}(k)^2}{|B|^2\tau_B(k^2)^2}\right)\mathrm{d}k$$

$$\geq \frac{1}{2}(2\pi)^{-3}\int_{(s\ell)^{-1}<|k|<R^{-1}} |k|^2\left(\sqrt{1+2\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}}-1-\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}+\frac{1}{2}\frac{n^2\widehat{W}(k)^2}{|B|^2\tau_B(k^2)^2}\right)\mathrm{d}k$$
$$- C(\rho a)^2\left[(\varepsilon_0+\varepsilon_T)\sqrt{\rho a}+(s\ell)^{-1}\ln\left(\sqrt{\rho a}s\ell\right)\right] - C(\rho a)^3\left((\varepsilon_0+\varepsilon_T)(\rho a)^{-\frac{1}{2}}+(s\ell)^{-1}(\rho a)^{-1}\right) \tag{132}$$

$$\geq \frac{1}{2}(2\pi)^{-3}\int_{(s\ell)^{-1}<|k|<R^{-1}} |k|^2\left(\sqrt{1+2\rho\widehat{v_R}(0)|k|^{-2}}-1-\rho\widehat{v_R}(0)|k|^{-2}+\frac{1}{2}\rho^2\widehat{v_R}(0)^2|k|^{-4}\right)\mathrm{d}k$$
$$- C(\rho a)^2\left[(\varepsilon_0+\varepsilon_T)\sqrt{\rho a}+(s\ell)^{-1}\ln\left(\sqrt{\rho a}s\ell\right)\right]$$
$$- C\int_{(s\ell)^{-1}<|k|<(\rho a)^{\frac{1}{2}}} |k|^2(\rho a)^2|k|^{-4}\left[\tfrac{1}{2}(kR)^2+C(\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{1}{2}}\right]\mathrm{d}k$$
$$- C\int_{(\rho a)^{\frac{1}{2}}<|k|<R^{-1}} |k|^2(\rho a)^3|k|^{-6}\left[\tfrac{1}{2}(kR)^2+C(\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{1}{2}}\right]\mathrm{d}k \tag{133}$$

$$\geq \frac{1}{2}(2\pi)^{-3}\int_{(s\ell)^{-1}<|k|<R^{-1}} |k|^2\left(\sqrt{1+2\rho\widehat{v_R}(0)|k|^{-2}}-1-\rho\widehat{v_R}(0)|k|^{-2}+\frac{1}{2}\rho^2\widehat{v_R}(0)^2|k|^{-4}\right)\mathrm{d}k$$
$$- C(\rho a)^2\left[(\varepsilon_0+\varepsilon_T)\sqrt{\rho a}+(s\ell)^{-1}\ln\left(\sqrt{\rho a}s\ell\right)\right]$$
$$- C(\rho a)^{\frac{5}{2}}\left((\rho a)^{\frac{1}{2}}R+(\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{1}{2}}\right). \tag{134}$$

In (132) we used that $\sqrt{1+2\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}}-1-\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}+\frac{1}{2}\frac{n^2\widehat{W}(k)^2}{|B|^2\tau_B(k^2)^2}$ is positive and can be bounded by $C(\rho a)^2|k|^{-4}$ if $|k|\leq(\rho a)^{\frac{1}{2}}$ and $C(\rho a)^3|k|^{-6}$ if $|k|\geq(\rho a)^{\frac{1}{2}}$. To arrive at (133), we note that if $f(x)=\sqrt{1+2x}-1-x+\frac{1}{2}x^2$, then $f'(x)=(1+2x)^{-\frac{1}{2}}-1+x$ and $0\leq\frac{1}{1+x}-1+x\leq f'(x)\leq\min\left\{x,\frac{3}{2}x^2\right\}$ for $x\geq 0$.
Recall that $|\frac{n}{|B|}-\rho|\leq C\rho\,(\rho a^3)^{\frac{1}{4}}\,\mathcal{S}_3{}^{\frac{1}{2}}$ by Lemma 6.4 and that $\widehat{W}(k)\geq(1-\frac{1}{2}(kR)^2)\int v_R(x)\,\mathrm{d}x$ by (88) if $|k|<R^{-1}$. Hence

$$\rho\widehat{v_R}(0)|k|^{-2}-\frac{n\widehat{W}(k)}{|B|\tau_B(k^2)}\leq\rho\frac{\widehat{v_R}(0)}{|k|^2}\left[\tfrac{1}{2}(kR)^2+C(\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{1}{2}}\right]. \tag{135}$$

We now note that

$$\frac{1}{2}(2\pi)^{-3}\int_{(s\ell)^{-1}<|k|<R^{-1}} |k|^2\left(\sqrt{1+2\rho\widehat{v_R}(0)|k|^{-2}}-1-\rho\widehat{v_R}(0)|k|^{-2}+\frac{1}{2}\rho^2\widehat{v_R}(0)^2|k|^{-4}\right)\mathrm{d}k \tag{136}$$

$$= \frac{1}{2}(2\pi)^{-3}(\rho\widehat{v_R}(0))^{\frac{5}{2}} \int\limits_{(s\ell)^{-1}(\rho\widehat{v_R}(0))^{-\frac{1}{2}}<|k|<R^{-1}(\rho\widehat{v_R}(0))^{-\frac{1}{2}}} -|k|^2 - 1 + |k|^2\sqrt{1+2|k|^{-2}} + \frac{1}{2}|k|^{-2}\,\mathrm{d}k \tag{137}$$

$$\geq 4\pi\rho^2 a\frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} - C(\rho a)^{\frac{5}{2}}[(s\ell)^{-1}(\rho a)^{-\frac{1}{2}} + R(\rho a)^{\frac{1}{2}}], \tag{138}$$

using that $a = 8\pi\widehat{v_R}(0) + O(R^{-1})$ and that $\int_{\mathbb{R}^3} -|k|^2 - 1 + |k|^2\sqrt{1+2|k|^{-2}} + \frac{1}{2}|k|^{-2}\,\mathrm{d}k = \frac{32}{15}\pi\sqrt{2}$ in (138), with the integrand being dominated by $\frac{1}{2}|k|^2$ if k is sufficiently small, respectively $C|k|^{-4}$, if $|k|$ is sufficiently large. From (A.16), respectively (A.4), (A.17) and (A.18), we obtain

$$\int\limits_{|k|<(s\ell)^{-1}} h_0(k)\,\mathrm{d}k|B|^{-1} + \int\limits_{|k|>R^{-1}} h_0(k)\,\mathrm{d}k|B|^{-1} \geq -C\rho a(s\ell)^{-3} - \frac{1}{4}(2\pi)^{-3}\int\limits_{|k|>R^{-1}} \frac{n^2}{|B|^2}\frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k - C(\rho a)^3 R. \tag{139}$$

Subtracting the term we added in (131) to the integral in (139) gives

$$-\frac{1}{4}(2\pi)^{-3}\int_{|k|>(s\ell)^{-1}} \frac{n^2}{|B|^2}\frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k, \tag{140}$$

which is related to the second Born term and is estimated using (A.22).

6.3 Final Bound for the Error Term

In this section we show that

$$\langle\widetilde{\psi}|-\varepsilon_0\Delta_u^{\mathcal{N}} + H_B|\widetilde{\psi}\rangle|B|^{-1} \geq 4\pi\rho^2\left(a_2 + \frac{128}{15\sqrt{\pi}}a((\rho a^3)^{1/2} + o((\rho a^3)^{1/2})\right) \tag{141}$$

with a_2 as in (8). In fact we obtain an explicit bound, which only depends on R and ρ. It then follows from (120) and Theorem 3.10 that Theorem 2.1 holds, which in turn implies our main Theorem 1.1.

We have accumulated quite a number of error-terms for the quantity $\langle\widetilde{\psi}|H_B|\widetilde{\psi}\rangle|B|^{-1}$ and these can be bounded by $C\rho^2 a\sqrt{\rho a^3}\mathcal{E}_i$ with

for (129): $\mathcal{E}_1 := \mathcal{S}_3\varepsilon_3^{-1}$

for (130): $\mathcal{E}_2 := \sum_{i=1}^{2}\mathcal{E}_2[i] := (\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{3}{2}} + \mathcal{S}_3(\rho|B|)^{-\frac{1}{2}}\mathcal{M}^{\frac{1}{2}}$

$$\text{for (134): } \mathcal{E}_3 := \sum_{i=1}^{5} \mathcal{E}_3[i] := \varepsilon_0 + \varepsilon_T + (\sqrt{\rho a} s\ell)^{-1} \ln(\sqrt{\rho a} s\ell) + (\rho a^3)^{\frac{1}{4}} \mathcal{S}_3^{\frac{1}{2}} + (\rho a)^{\frac{1}{2}} R$$

$$\text{for (138): } \mathcal{E}_4 := \sum_{i=1}^{2} \mathcal{E}_4[i] := (\rho a)^{-\frac{1}{2}} (s\ell)^{-1} + (\rho a)^{\frac{1}{2}} R$$

$$\text{for (139): } \mathcal{E}_5 := \sum_{i=1}^{2} \mathcal{E}_5[i] := (\rho a)^{-\frac{3}{2}} (s\ell)^{-3} + (\rho a)^{\frac{1}{2}} R$$

$$\text{for (A.22): } \mathcal{E}_6 := \sum_{i=1}^{3} \mathcal{E}_6[i] := (\rho a^3)^{-\frac{1}{2}} \frac{a}{R} \varepsilon_0 + (\rho a)^{-\frac{1}{2}} (s\ell)^{-1} \ln\left(\frac{s\ell}{R}\right) + (\rho a^3)^{-\frac{1}{2}} \varepsilon_T \frac{a}{ds\ell} \ln\left(\frac{ds\ell}{R}\right).$$

We now arrive at

$$\frac{1}{2}(2\pi)^{-3} \int\limits_{k\in\mathbb{R}^3} h_0(k)\,\mathrm{d}k|B|^{-1} \geq -\frac{1}{4}(2\pi)^{-3}\rho^2 \int \frac{\widehat{v_R}(k)^2}{|k|^2}\,\mathrm{d}k + 4\pi\rho^2 a \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3}$$
$$- C\rho^2 a \sqrt{\rho a^3}\,(\mathcal{E}_3 + \mathcal{E}_4 + \mathcal{E}_5 + \mathcal{E}_6)\,. \tag{142}$$

Further we introduce

$$\text{for (85): } \mathcal{E}_7 := \mathcal{S}_3\,(\rho|B|)^{-1}$$

$$\text{for (90): } \mathcal{E}_8 := \mathcal{S}_3 (R/\ell)^{2M}$$

$$\text{for (120): } \mathcal{E}_9 := \mathcal{M}^{-2} (\rho a^3)^{-\frac{1}{2}} \frac{a}{R}$$

$$\text{all errors: } \mathcal{E}_{\text{total}} := \sum_{i=1}^{9} \mathcal{E}_i.$$

With the above notation we obtain using Condition 1, (120), Lemmas 6.2 and 6.4 that

$$\langle \Psi | -\varepsilon_0 \Delta_u^{\mathcal{N}} + H_B | \Psi \rangle |B|^{-1} \geq 4\pi\rho^2 \left(a_2 + \frac{128}{15\sqrt{\pi}} a \left((\rho a^3)^{\frac{1}{2}} - C\mathcal{E}_{\text{total}} \right) \right). \tag{143}$$

All contributions to $\mathcal{E}_{\text{total}}$ can be chosen to be of order $o(1)$. By choosing our parameters carefully, we find an explicit upper bound for $\mathcal{E}_{\text{total}}$ in terms of ρ, R and a. We choose

$$\varepsilon_3 := c_3 \varepsilon_0 \frac{R}{a} \mathcal{M}^{-1}, \tag{144}$$

where c_3 is a small universal constant, which ensures that the requirement in Lemma 6.6 is satisfied. Observe that only the error terms

$$\varepsilon_0 (\rho a^3)^{-\frac{1}{2}} \frac{a}{R} \qquad \text{and} \qquad \mathcal{S}_3 \varepsilon_3^{-1} = c_3^{-1} \mathcal{S}_3 \varepsilon_0^{-1} \frac{a}{R} \mathcal{M} \tag{145}$$

depend on ε_0. We choose

$$\varepsilon_0 := \mathcal{S}_3^{\frac{1}{2}}(\rho a^3)^{\frac{1}{4}}\mathcal{M}^{\frac{1}{2}}, \tag{146}$$

since then

$$\mathcal{E}_1 = \mathcal{S}_3\varepsilon_3^{-1} = c_3^{-1}\mathcal{S}_3\frac{a}{R}\varepsilon_0^{-1}\mathcal{M} = C(\rho a^3)^{-\frac{1}{2}}\frac{a}{R}\varepsilon_0 = \mathcal{E}_6[1]. \tag{147}$$

We choose ε_T as small as possible without violating Condition 3 by setting

$$\varepsilon_T := c_T^{-1}(\sqrt{\rho a}d\ell)^2. \tag{148}$$

Recall that the term $\varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R}$ appears in $\mathcal{S}_2$. With ε_0 as in (146) we have

$$\varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R} = \mathcal{S}_3^{\frac{1}{2}}(\rho a^3)^{-\frac{1}{4}}\frac{a}{R}\mathcal{M}^{\frac{1}{2}}. \tag{149}$$

We impose the following condition.

CONDITION 7: *We require that*

$$\varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R} \leq (\sqrt{\rho a}ds\ell)^{-3}. \tag{150}$$

Applying Condition 1 and 7, we may write

$$\mathcal{S}_2 = (\sqrt{\rho a}ds\ell)^{-3}, \tag{151}$$

$$\mathcal{S}_3 = \mathcal{S}_2\rho a\ell^2 = (\rho a^3)^{-\frac{1}{2}}\left(\frac{ds\ell}{a}\right)^{-3}\left(\frac{\ell}{a}\right)^2, \tag{152}$$

where $\mathcal{S}_2$ is the quantity introduced in (113), which collects the error terms that we obtained on the small box. Note that this is a weak condition, since $\varepsilon_0(\rho a^3)^{-\frac{1}{2}}\frac{a}{R}$ also appears as the error term $\mathcal{E}_6[1]$. Condition 5 (ii) requires that we choose

$$\mathcal{M} \geq \rho|B|\sqrt{\rho a^3}\mathcal{S}_3 = \rho a^3\left(\frac{\ell}{a}\right)^5\left(\frac{a}{ds\ell}\right)^3. \tag{153}$$

In fact we will choose $\mathcal{M}$ even larger if R is small, since otherwise the term $\mathcal{E}_9$ will be large. That Condition 5 (i) holds, follows from Condition 1 when we show that the error term $\mathcal{E}_9$ is small, since

$$\frac{a}{R}\mathcal{M}^{-2} = (\rho a^3)^{\frac{1}{2}}\mathcal{E}_9.$$

From (153) we have

$$\mathcal{E}_2 = (\rho a^3)^{\frac{1}{4}}\mathcal{S}_3^{\frac{3}{2}} + \mathcal{S}_3(\rho|B|)^{-\frac{1}{2}}\mathcal{M}^{\frac{1}{2}} \leq 2\mathcal{S}_3(\rho|B|)^{-\frac{1}{2}}\mathcal{M}^{\frac{1}{2}}. \tag{154}$$

By Condition 1 it is clear that $\mathcal{E}_5 \leq \mathcal{E}_4 \leq \mathcal{E}_3$ and with the choice for ε_T in (148) we obtain

$$\begin{aligned}\mathcal{E}_3[5] = \sqrt{\rho a}R &= c_T\sqrt{\rho a}R(\sqrt{\rho a}d\ell)^{-2}\varepsilon_T \\ &= c_T(\rho a^3)^{-\frac{1}{2}}s^2R\left(\frac{a}{ds\ell}\right)^2\varepsilon_T \\ &< \delta c_T s^2(\rho a^3)^{-\frac{1}{2}}\frac{a}{ds\ell}\varepsilon_T\ln\left(\frac{ds\ell}{R}\right) \leq \mathcal{E}_6[3].\end{aligned} \tag{155}$$

Thus $\mathcal{E}_3 \leq \mathcal{E}_6 + \mathcal{E}_2[1]$. By Condition 1 $\rho^{-\frac{1}{3}} < \delta ds\ell$ and hence

$$\mathcal{E}_7 = (\sqrt{\rho a}ds\ell)^{-3}\frac{a}{\ell} < \delta^3 s(\rho a)^{-\frac{1}{2}}(s\ell)^{-1} \leq \mathcal{E}_4[1]. \tag{156}$$

Since we chose $M \geq 2$, it follows, again from Condition 1, that

$$\mathcal{E}_8 = \mathcal{S}_3(R/\ell)^{2M} \leq \mathcal{S}_3(R/\ell)^4 = \left(\rho a^3\right)^{-\frac{1}{2}}\left(\frac{a}{\ell}\right)^2 R\left(\frac{R}{ds\ell}\right)^3 < \delta^5 s^2(\rho a)^{\frac{1}{2}}R. \tag{157}$$

We are left with error terms of order

$$\begin{aligned}&\left(\frac{ds\ell}{a}\right)^{-\frac{3}{2}}(\rho a^3)^{-\frac{1}{2}}\frac{\ell}{a}\frac{a}{R}\mathcal{M}^{\frac{1}{2}} + (\rho a^3)^{-1}\left(\frac{ds\ell}{a}\right)^{-3}\left(\frac{\ell}{a}\right)^{\frac{1}{2}}\mathcal{M}^{\frac{1}{2}} \\ &+ (\rho a)^{-\frac{1}{2}}(s\ell)^{-1} + (\rho a)^{\frac{1}{2}}s^{-1}d\ell + (\rho a^3)^{-\frac{1}{2}}\frac{a}{R}\mathcal{M}^{-2}.\end{aligned} \tag{158}$$

Note that $\left(\frac{ds\ell}{a}\right)^{-\frac{3}{2}}(\rho a^3)^{-\frac{1}{2}}\frac{\ell}{a} > \delta^{-1}(\rho a^3)^{-\frac{1}{4}}$ by Condition 1. Optimizing over $\mathcal{M}$ shows that we have to require $\lim_{\rho\to 0} R\rho^{-\frac{1}{3}}(\rho a^3)^{\frac{1}{30}} = 0$. This is why we have $\eta = \frac{1}{30}$ in our main theorem 1.1.

The first term in (158) is larger than the second term if

$$\frac{a}{R} \geq (\rho a^3)^{-\frac{1}{2}}\left(\frac{ds\ell}{a}\right)^{-\frac{3}{2}}\left(\frac{\ell}{a}\right)^{-\frac{1}{2}}. \tag{159}$$

Note that (159) holds if $\frac{R}{a}$ is close to $(\rho a^3)^{-\frac{3}{10}}$ and we therefore have to choose $ds\ell$ and ℓ close to $(\rho a)^{-\frac{1}{2}}$. In Condition 5 we required that $\mathcal{M} \geq (\sqrt{\rho a}\ell)^3\mathcal{S}_3 = (\rho a^3)\left(\frac{ds\ell}{a}\right)^{-3}\left(\frac{\ell}{a}\right)^5$. For small R it is advantageous to choose $\mathcal{M}$ larger than this bound.

We use the following choices for $\mathcal{M}$:

$$\mathcal{M}_1 = \left(\frac{ds\ell}{a}\right)^{\frac{3}{5}} \left(\frac{\ell}{a}\right)^{-\frac{2}{5}}, \quad \mathcal{M}_2 = \rho a^3 \left(\frac{ds\ell}{a}\right)^{-3} \left(\frac{\ell}{a}\right)^{5}, \quad \mathcal{M}_3 = (\rho a^3)^{\frac{1}{5}} \left(\frac{ds\ell}{a}\right)^{\frac{6}{5}} \left(\frac{\ell}{a}\right)^{-\frac{1}{5}} \left(\frac{a}{R}\right)^{\frac{2}{5}}.$$

6.4 Choices for the Parameters d, s, and ℓ

Up to a constant factor we will choose our parameters in the following way.

Case I:

If $\frac{R}{a} \leq (\rho a^3)^{-\frac{1}{9}\frac{3M+5}{M+2}}$, we choose

$$d = (\rho a^3)^{\frac{-3M+6}{15M-20}} \left(\frac{R}{a}\right)^{\frac{-2M+4}{3M-4}}, \qquad s = (\rho a^3)^{\frac{-3}{3M-4}} \left(\frac{R}{a}\right)^{\frac{-10}{3M-4}}, \qquad \frac{\ell}{a} = (\rho a^3)^{\frac{-6M+7}{15M-20}} \left(\frac{R}{a}\right)^{\frac{M-2}{3M-4}},$$

such that $ds^{\frac{-M+2}{5}} = 1$, $ds\ell > \rho^{-\frac{1}{3}}$ and, since $\frac{R}{a} > (\rho a^3)^{-\frac{3}{10}}$, also $s < 1, d\ell < (\rho a)^{-\frac{1}{2}} < s\ell$. (159) holds with this choice of parameters provided $\frac{R}{a} \leq (\rho a^3)^{-\frac{1}{10}\frac{18M+19}{4M+9}}$. We have that $\mathcal{M}_1 \geq \mathcal{M}_2$ if $\frac{R}{a} \leq (\rho a^3)^{-\frac{1}{9}\frac{3M+5}{M+2}}$. For the error terms we obtain the bound

$$\left[(\rho a^3)^{-\frac{3}{10}} \left(\frac{a}{R}\right)\right]^{\frac{M-12}{3M-4}}. \tag{160}$$

Case II:

If $(\rho a^3)^{-\frac{1}{9}\frac{3M+5}{M+2}} \leq \frac{R}{a} \leq (\rho a^3)^{-\frac{1}{2}\frac{16M+23}{17M+36}}$, we choose

$$d = (\rho a^3)^{\frac{-M+2}{15M+10}} \left(\frac{R}{a}\right)^{\frac{-4M+8}{15M+10}}, \qquad s = (\rho a^3)^{-\frac{1}{3M+2}} \left(\frac{R}{a}\right)^{-\frac{4}{3M+2}}, \qquad \frac{\ell}{a} = (\rho a^3)^{-\frac{7M+6}{15M+10}} \left(\frac{R}{a}\right)^{\frac{2M-4}{15M+10}}.$$

We have $ds^{\frac{-M+2}{5}} = 1$, $ds\ell > \rho^{-\frac{1}{3}}$ and, since $\frac{R}{a} > (\rho a^3)^{-\frac{1}{4}}$, also $s < 1, d\ell < (\rho a)^{-\frac{1}{2}} < s\ell$. Note that $ds\ell > R$ if $\frac{R}{a} < (\rho a^3)^{-\frac{8M+9}{17M+26}}$. Equation (159) holds with this choice of parameters provided $\frac{R}{a} \leq (\rho a^3)^{-\frac{1}{2}\frac{16M+23}{17M+36}}$. We have that $\mathcal{M}_1 \leq \mathcal{M}_2$ if $\frac{R}{a} \geq (\rho a^3)^{-\frac{1}{9}\frac{3M+5}{M+2}}$. Note that $(\rho a^3)^{-\frac{1}{9}\frac{3M+5}{M+2}} < (\rho a^3)^{-\frac{1}{2}\frac{16M+23}{17M+36}} < (\rho a^3)^{-\frac{8M+9}{17M+26}}$. For the error terms we obtain the bound

$$\left[(\rho a^3)^{\frac{1}{2}} \left(\frac{R}{a}\right)^2\right]^{\frac{-M+12}{15M+10}}. \tag{161}$$

Case III:

If $(\rho a^3)^{-\frac{1}{2}\frac{16M+23}{17M+36}} \leq \frac{R}{a} \leq (\rho a^3)^{-\frac{8M+14}{17M+36}}$, we choose

$$d = (\rho a^3)^{\frac{M-2}{17M+36}}, \qquad s = (\rho a^3)^{\frac{5}{17M+36}}, \qquad \frac{\ell}{a} = (\rho a^3)^{-\frac{9M+17}{17M+36}},$$

such that $R \leq ds\ell$ provided $\frac{R}{a} \leq (\rho a^3)^{-\frac{8M+14}{17M+36}}$. It is easy to check that the other equations in Condition 1 hold. Equation (159) does not hold with this choice, provided $\frac{R}{a} \geq (\rho a^3)^{-\frac{1}{2}\frac{16M+23}{17M+36}}$. For the error terms we obtain

$$(\rho a^3)^{\frac{1}{2}\frac{M-12}{17M+36}}.$$

Case IV:

If $\frac{R}{a} \geq (\rho a^3)^{-\frac{8M+14}{17M+36}}$, we choose

$$d = (\rho a^3)^{\frac{M-2}{M+8}} \left(\frac{R}{a}\right)^{\frac{2M-4}{M+8}}, \qquad s = (\rho a^3)^{\frac{5}{M+8}} \left(\frac{R}{a}\right)^{\frac{10}{M+8}}, \qquad \frac{\ell}{a} = (\rho a^3)^{-\frac{M+3}{M+8}} \left(\frac{R}{a}\right)^{\frac{-M+2}{M+8}}.$$

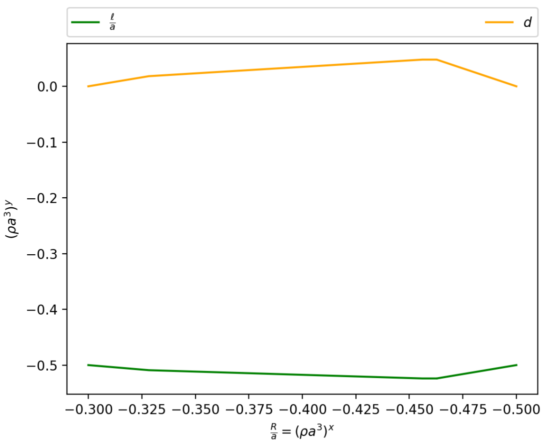
It is easy to check that Condition 1 holds. Equation (159) does not hold. We choose $\mathcal{M}_2$ if $(\rho a^3)^{-\frac{8M+14}{17M+36}} \leq \frac{R}{a} \leq (\rho a^3)^{-\frac{2}{5}\frac{11M+23}{9M+20}}$. For $\frac{R}{a} \geq (\rho a^3)^{-\frac{2}{5}\frac{11M+23}{9M+20}}$ we may choose $\mathcal{M}_3$. For the error terms we obtain

$$\left[(\rho a^3)^{\frac{1}{2}} \left(\frac{R}{a}\right)\right]^{\frac{M-12}{M+8}}.$$

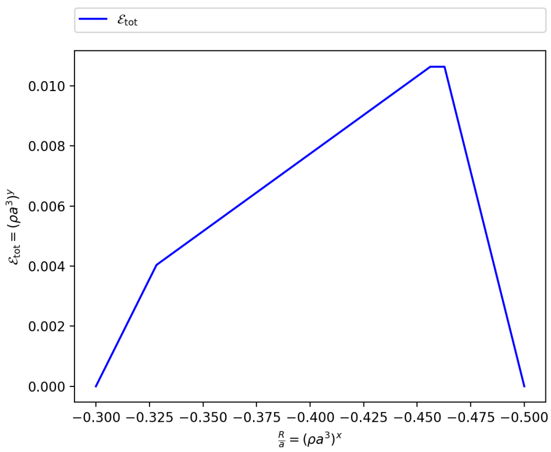
This completes the bound on the error term ω in Theorem 2.1.

6.4.1 Graphs

Note that if R is of the form $\frac{R}{a} = (\rho a^3)^x$, then we can write $\mathcal{E}_{\text{total}} = (\rho a^3)^y$ with y depending on x. The same holds for our choice of d and $\frac{\ell}{a}$. See Figure 1.



(a) $\frac{\ell}{a}$ and d depending on R.



(b) $\mathcal{E}_{\text{total}}$ depending on R.

Figure 1: *Choice of parameters and estimate on the error term $\mathcal{E}_{\text{total}}$ depending on R for $M = 20$. The graphs have been produced using Pythons matplotlib and numpy packages.*

Our choices for our parameters depend on the choice of M due to Condition 2. As M increases, the bound on $\mathcal{E}_{\text{total}}$ is improved and the range of the plateau corresponding to Case III above becomes small.

A Appendix

Throughout this appendix we will assume that $n \geq 1$ and that the condition on $n|B|^{-1}$ in Lemma 4.6 is satisfied, so that by Lemma 4.4 we have the lower bounds

$$H_{\text{Quad}} \geq \frac{1}{2}(2\pi)^{-3} \int_{\mathbb{R}^3} h_0(k)\, \mathrm{d}k - Cn_+ a \min\{R^{-3}, |B|^{-1}\} \max \chi_B^2$$

and

$$h_0(k) \geq -\left(n^{-1}\tau_B(k^2) + |B|^{-1}\widehat{W}(k) - \sqrt{n^{-2}\tau_B(k^2)^2 + 2n^{-1}|B|^{-1}\tau_B(k^2)\widehat{W}(k)} \right) n_0 \int \chi_B^2. \tag{A.1}$$

A.1 Bounds for the Quadratic Part of H_B

We estimate the operator valued integral $\frac{1}{2}(2\pi)^{-3}\int h_0(k)\,\mathrm{d}k$ using the following facts. Around $x = 0$ we can write $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3 + O(x^4)$ yielding the bounds

$$1 + \frac{1}{2}x - Cx^2 \leq \sqrt{1+x} \leq 1 + \frac{1}{2}x - \frac{1}{8}x^2 + Cx^3 \tag{A.2}$$

$$\sqrt{1+x} \geq 1 + \frac{1}{2}x - \frac{1}{8}x^2 \qquad \text{(if and only if } x \geq 0) \tag{A.3}$$

$$1 + \frac{1}{2}x - \frac{1}{8}x^2 - Cx^3 \leq \sqrt{1+x} \leq 1 + \frac{1}{2}x. \tag{A.4}$$

If B is either a small or a large box, we have for all $k \in \mathbb{R}^3$ that

$$h_0(k) \leq 0. \tag{A.5}$$

This is easy to see. If B is a small box and $|k| \leq (ds\ell)^{-1}$, then $\tau_B(k^2) = 0$ and $\widehat{W}(k) > 0$ by (88) since $(ds\ell)^{-1} < R^{-1}$. For $|k| > (ds\ell)^{-1}$ we use (A.4). For the large box the claim is proven analogously. We may therefore replace n_0 by n in (A.1) when bounding h_0 from below.

A.1.1 Estimates on the Small Box

$\tau_B(k^2) = 0$ if $|k| < (ds\ell)^{-1}$ while $\widehat{W}(k) > 0$ if $|k| < R^{-1}$. Since $\sqrt{1+x} \geq 1$ if $x \geq 0$, we have

$$\int\limits_{|k|<2(ds\ell)^{-1}} h_0(k)\,\mathrm{d}k \geq -\int\limits_{|k|<2(ds\ell)^{-1}} \frac{n_0}{|B|}\widehat{W}(k)\,\mathrm{d}k \int \chi_B^2 \geq -C\frac{n}{|B|}a(ds\ell)^{-3}\int \chi_B^2. \tag{A.6}$$

Using (A.3) for $2(ds\ell)^{-1} < |k| < R^{-1}$ and (A.4) for $|k| > R^{-1}$ gives

$$\frac{1}{2}(2\pi)^{-3} \int\limits_{|k|>2(ds\ell)^{-1}} h_0(k)\,\mathrm{d}k \geq \frac{1}{2}(2\pi)^{-3} \int\limits_{|k|>2(ds\ell)^{-1}} -\frac{1}{2}\frac{n^2}{|B|^2}\frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k \int \chi_B^2 - C \int\limits_{|k|>R^{-1}} \frac{n^3}{|B|^3}\frac{\widehat{W}(k)^3}{\tau_B(k^2)^2}\,\mathrm{d}k \int \chi_B^2. \tag{A.7}$$

Since $\tau_B = (1-\varepsilon_0)[|k| - (ds\ell)^{-1}]_+^2 \geq C|k|^2$ if $|k| \geq 2(ds\ell)^{-1}$ and $|\widehat{W}(k)| \leq \widehat{W}(0) \leq Ca$, it is easy to estimate the last term in (A.7)

$$\int\limits_{|k|>R^{-1}} \frac{n^3}{|B|^3}\frac{\widehat{W}(k)^3}{\tau_B(k^2)^2} \int \chi_B^2\,\mathrm{d}k \leq C \int\limits_{|k|>R^{-1}} \frac{n^3}{|B|^3}\frac{a^3}{|k|^4}\,\mathrm{d}k \int \chi_B^2 \leq C\frac{n^3}{|B|^3}a^3 R \int \chi_B^2. \tag{A.8}$$

The integral $\int\limits_{|k|>2(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k$ is related to the second Born term and we have to estimate it carefully. On the small box we have $v_R(x) \leq W(x) \leq v_R(x)(1 + C(\frac{x}{d\ell})^2)$, as explained on page 11, such that

$$||v_R - W||_{\frac{6}{5}} \leq C(\tfrac{R}{d\ell})^2 ||v_R||_{\frac{6}{5}}. \tag{A.9}$$

Since $v_R(x) = \frac{1}{R^3}v_1(\frac{x}{R})$, we have $\widehat{v_R}(k) = \widehat{v}_1(Rk)$ and that

$$\int_{|k|\geq 2(ds\ell)^{-1}} \frac{\widehat{v_R}(k)^2}{|k|^2}\,\mathrm{d}k = \frac{1}{R}\int_{|k|\geq 2(ds\ell)^{-1}R} \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k. \tag{A.10}$$

Note that

$$||v_R||_{\frac{6}{5}} = R^{-\frac{1}{2}} ||v_1||_{\frac{6}{5}}$$

and for $f \in L^{\frac{6}{5}}(\mathbb{R}^3)$ by the Hardy-Littlewood-Sobolev inequality (see [20] Cor 5.10) we have

$$\int |\widehat{f}(k)|^2 |k|^{-2}\,\mathrm{d}k \leq C||f||_{\frac{6}{5}}. \tag{A.11}$$

On the small box we have for $|k| > 2(ds\ell)^{-1}$

$$\tau_B(k^2)^{-1} \leq (1 + C\varepsilon_0)|k|^{-2} + C(ds\ell)^{-1}|k|^{-3}. \tag{A.12}$$

We use the Cauchy-Schwarz inequality (A.9) and (A.11) to obtain the estimate

$$\begin{aligned}\int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^2}\,\mathrm{d}k \leq& \int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{v}_R(k)^2}{|k|^2}\,\mathrm{d}k \\ &+ 2\left(\int_{|k|>2(ds\ell)^{-1}} \frac{|\widehat{W}(k)-\widehat{v}_R(k)|^2}{|k|^2}\,\mathrm{d}k\right)^{\frac{1}{2}}\left(\int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{v}_R(k)^2}{|k|^2}\,\mathrm{d}k\right)^{\frac{1}{2}} \\ &+ \int_{|k|>2(ds\ell)^{-1}} \frac{|\widehat{W}(k)-\widehat{v}_R(k)|^2}{|k|^2}\,\mathrm{d}k \\ \leq& \frac{1}{R}\int_{|k|>2(ds\ell)^{-1}R} \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k + C||W-v_R||_{\frac{6}{5}}||v_R||_{\frac{6}{5}} + C||W-v_R||^2_{\frac{6}{5}} \\ \leq& \frac{1}{R}\int_{|k|>2(ds\ell)^{-1}R} \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k + C\left(\frac{R}{d\ell}\right)^2\frac{a^2}{R}. \qquad \text{(A.13)}\end{aligned}$$

Using $|\widehat{W}(k)| \leq Ca$, gives

$$\begin{aligned}\int_{|k|>2(ds\ell)^{-1}} \widehat{W}(k)^2\,|k|^{-3}\,\mathrm{d}k =& \int_{2(ds\ell)^{-1}<|k|<R^{-1}} \widehat{W}(k)^2|k|^{-3}\,\mathrm{d}k + \int_{|k|>R^{-1}} \widehat{W}(k)^2\,|k|^{-3}\,\mathrm{d}k \\ \leq& C\int_{2(ds\ell)^{-1}R<|k|<1} \widehat{W}(0)^2|k|^{-3}\,\mathrm{d}k + R\int_{|k|>2(ds\ell)^{-1}} \widehat{W}(k)^2\,|k|^{-2}\,\mathrm{d}k \\ \leq& Ca^2\ln\left(\frac{ds\ell}{R}\right) + R\int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^2}\,\mathrm{d}k \\ \leq& Ca^2\ln\left(\frac{ds\ell}{R}\right). \qquad \text{(A.14)}\end{aligned}$$

Combining (A.12), (A.13) and (A.14), we arrive at

$$\begin{aligned}\int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k \leq& (1+C\varepsilon_0)\int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^2}\,\mathrm{d}k + C(ds\ell)^{-1}\int_{|k|>2(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^3}\,\mathrm{d}k \\ \leq& (1+C\varepsilon_0)\frac{1}{R}\int \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k + Ca\frac{a}{ds\ell}\ln\left(\frac{ds\ell}{R}\right). \qquad \text{(A.15)}\end{aligned}$$

In the last inequality we used that the second term in (A.13) and the positive term $(1+C\varepsilon_0)\frac{1}{R}\int_{|k|<2(ds\ell)^{-1}R} \frac{\widehat{v}_1(k)^2}{|k|^2}\,\mathrm{d}k$ by Condition 1 are bounded by the last term in (A.15).

A.1.2 Estimates on the Large Box

On the large box we have $\tau_B(k^2) = (1-\varepsilon_0)(1-\varepsilon_T)\ \left[|k| - \frac{1}{2}(s\ell)^{-1}\right]_+^2 + (1-\varepsilon_0)\varepsilon_T\ \left[|k| - \frac{1}{2}(ds\ell)^{-1}\right]_+^2$ and $\int \chi_B^2 = |B|$. Hence

$$\int\limits_{|k|<(s\ell)^{-1}} h_0(k)\,\mathrm{d}k \geq -\int\limits_{|k|<(s\ell)^{-1}} \frac{n_0}{|B|}\widehat{W}(k)\,\mathrm{d}k \int \chi_B^2 \geq -C\frac{n}{|B|}a(s\ell)^{-3}|B|. \tag{A.16}$$

Analogously to (A.7) we have

$$\frac{1}{2}(2\pi)^{-3}\int\limits_{|k|>(s\ell)^{-1}} h_0(k)\,\mathrm{d}k \geq \frac{1}{2}(2\pi)^{-3}\int\limits_{|k|>(s\ell)^{-1}} -\frac{1}{2}\frac{n^2}{|B|^2}\frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k|B| - C\int\limits_{|k|>R^{-1}} \frac{n^3}{|B|^3}\frac{\widehat{W}(k)^3}{\tau_B(k^2)^2}\,\mathrm{d}k|B|. \tag{A.17}$$

The last term in (A.17) is estimated in the same way as the last term in (A.7)

$$\int\limits_{|k|>R^{-1}} \frac{n^3}{|B|^3}\frac{\widehat{W}(k)^3}{\tau_B(k^2)^2}\int \chi_B^2\,\mathrm{d}k \leq C\int\limits_{|k|>R^{-1}} \frac{n^3}{|B|^3}\frac{a^3}{|k|^4}\,\mathrm{d}k|B| \leq C\frac{n^3}{|B|^3}a^3R|B|. \tag{A.18}$$

On the large box we have $v_R(x) \leq W(x) \leq v_R(x)(1 + C(\frac{x}{\ell})^2)$ and therefore, similarly to (A.13),

$$\int_{|k|>(s\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^2}\,\mathrm{d}k \leq \int_{|k|>(s\ell)^{-1}} \frac{\widehat{v}_R(k)^2}{|k|^2}\,\mathrm{d}k + C\frac{a^2R}{\ell^2}. \tag{A.19}$$

Similarly to (A.14) we have

$$\int_{|k|>(s\ell)^{-1}} \widehat{W}\,(k)^2\,|k|^{-3}\,\mathrm{d}k \leq Ca^2\ln\left(\frac{s\ell}{R}\right). \tag{A.20}$$

Since

$$\tau_B(k^2)^{-1} \leq \begin{cases} (1 + C\varepsilon_0 + C\varepsilon_T)\,|k|^{-2} + C(s\ell)^{-1}|k|^{-3} & \text{for } (s\ell)^{-1} < |k| < (ds\ell)^{-1} \\ (1 + C\varepsilon_0)\,|k|^{-2} + C\left((s\ell)^{-1} + \varepsilon_T(ds\ell)^{-1}\right)|k|^{-3} & \text{for } |k| \geq (ds\ell)^{-1}, \end{cases} \tag{A.21}$$

we have

$$\int_{|k|>(s\ell)^{-1}} \frac{\widehat{W}(k)^2}{\tau_B(k^2)}\,\mathrm{d}k \leq (1 + C\varepsilon_0 + C\varepsilon_T)\int_{(s\ell)^{-1}<|k|<(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^2} + C(s\ell)^{-1}\frac{\widehat{W}(k)^2}{|k|^3}\,\mathrm{d}k$$

$$
\begin{aligned}
&+ (1 + C\varepsilon_0) \int_{|k|>(ds\ell)^{-1}} \frac{\widehat{W}(k)^2}{|k|^2} + C\left((s\ell)^{-1} + \varepsilon_T (ds\ell)^{-1}\right) \frac{\widehat{W}(k)^2}{|k|^3} \,\mathrm{d}k \\
\leq\ & \int_{|k|>(s\ell)^{-1}} \frac{\widehat{v_R}(k)^2}{|k|^2} \,\mathrm{d}k + C\varepsilon_0 a \frac{a}{R} + C\frac{a^2 R}{\ell^2} + C\epsilon_T a^2 (ds\ell)^{-1} \\
&+ C(s\ell)^{-1} a^2 \ln\left(\frac{s\ell}{R}\right) + C\varepsilon_T (ds\ell)^{-1} a^2 \ln\left(\frac{ds\ell}{R}\right) \\
\leq\ & \int \frac{\widehat{v_R}(k)^2}{|k|^2} \,\mathrm{d}k + C\varepsilon_0 a \frac{a}{R} + C(s\ell)^{-1} a^2 \ln\left(\frac{s\ell}{R}\right) \\
&+ C\varepsilon_T (ds\ell)^{-1} a^2 \ln\left(\frac{ds\ell}{R}\right). \qquad \text{(A.22)}
\end{aligned}
$$

In the last inequality we used that $C\frac{aR}{\ell^2}a$ and the positive term $\int_{|k|<(s\ell)^{-1}} \frac{\widehat{v}_R(k)^2}{|k|^2} \,\mathrm{d}k$ by Condition 1 are bounded by the second to last term in (A.22).

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