Master's Thesis

in Theoretical and Mathematical Physics

Ludwig-Maximilians-Universität München

Department Mathematisches Institut

A Second Order Ground State Energy Expansion for the Dilute Bose Gas

Marcel Oliver Schaub

September 4, 2017

supervised by:
Prof. PhD Thomas Østergaard Sørensen

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Abstract

We prove a two-term asymptotics for the canonical zero-temperature Bogolubov energy functional. The functional describes a homogeneous, dilute gas of repulsively interacting Bosons in 3 spatial dimensions in the thermodynamic limit. As a main result, we show the formula $4\pi a\rho^2 + \frac{512\sqrt{\pi}}{15} C \cdot (\rho a)^{5/2} + \mathrm{o}(\rho a)^{5/2}$ for the ground state energy density as $\rho a \to 0$. Here, ρ is the density of the gas and a is the scattering length of the two-body interaction potential V. The explicit constant $C > 1$ is depending on the potential. The result is in agreement with the upper bound given by [1] and the method is inspired by [3]. The second order term carries a constant which is strictly larger than the one in the Lee-Huang-Yang formula.

Contents

1 Introduction and Main Result

The physical phenomenon of Bose-Einstein condensation has been intensively studied in the past and present century. First discovered by A. Einstein in 1925 [6], it soon became a great challenge for both physicists and mathematicians. In particular, proving existence of Bose-Einstein condensation for real, interacting gases turned out to be beyond reach for the existing methods until the present day. Nevertheless, the are efforts to treat the problem systematically. In this thesis, we give the proof of an asymptotic formula for the ground state energy of an interacting Bose gas in the low-density limit.

1.1 The interacting Bose gas on a finite box

A gas of N identical and pairwise interacting bosons in 3 spatial dimensions is, in suitable units, described by the Hamiltonian

$$H_{N,L} := -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leqslant i < j \leqslant N} V(x_i - x_j). \tag{1.1}$$

It consists of the kinetic energy and the two-particle interaction term given by $V: \mathbb{R}^3 \to \mathbb{R}$. The physical space is the open cubic box $\Lambda_L := (-L/2, L/2)^3$ of side length $L > 0$. This means that $H_{N,L}$ is acting in the bosonic N-particle Hilbert space $\mathcal{H}_{N,L} = L^2_{\mathrm{sym}}(\Lambda_L^N)$ of square-integrable functions Ψ, which are symmetric with respect to permutation of their coordinates. For a complete setup, one has to specify boundary conditions, which can be either Dirichlet, Neumann, or periodic. The Hamiltonian $H_{N,L}$ can be properly realized as a self-adjoint operator with dense domain $\mathcal{D}(H_{N,L}) \subseteq \mathcal{H}_{N,L}$ by Friedrichs' method. We refer to [4, p.2] for more details. As usual, the ground state energy $E_{N,L}$ of $H_{N,L}$ is the infimum of the spectrum:

$$E_{N,L} := \inf\{\langle \Psi, H_{N,L}\Psi\rangle_{\mathcal{H}_{N,L}} : \Psi \in \mathcal{D}(H_{N,L}),\ \|\Psi\|_{\mathcal{H}_{N,L}} = 1\}. \tag{1.2}$$

If $\Psi_0 \in \mathcal{H}_{N,L}$ exists such that

$$E_{N,L} = \langle \Psi_0, H_{N,L}\Psi_0\rangle_{\mathcal{H}_{N,L}},$$

we call Ψ_0 a ground state of $H_{N,L}$. Generally, if it exists, one would like to gain structural information on the ground state Ψ_0. This also contains the question whether Ψ_0 is a Bose-Einstein condensate state. This, in turn, requires a suitable definition of Bose-Einstein condensation in advance. It turns out that the obvious definition for the ideal gas may not easily be generalized for interacting systems, see Subsection 1.2.

In most cases, the "microscopic" information – how Ψ_0 and $E_{N,L}$ depend on N and L – is far from known. Typically, N is very large and so the system is too complicated. However, making use of that, we can consider the mean particle density $\rho := \frac{N}{L^3} \geqslant 0$ instead. Then, one intends to extract partial information for (1.2) by considering the macroscopic, or thermodynamic, limit $(N, L) = (\rho L^3, L) \to \infty$. This means that we take $N, L \to \infty$ simultaneously, keeping the density ρ fixed. This motivates the definition of the ground state energy density as a function of ρ by

$$e_0(\rho) := \lim_{L\to\infty} \frac{E_{\rho L^3, L}}{\rho L^3}. \tag{1.3}$$

1.2 Historical development

For the ideal gas, the Hamiltonian is $H_{N,L}$ from (1.1) with $V \equiv 0$. In this case, Bose-Einstein condensation was introduced and proved by Einstein in [6]. His observation was that the ground state of $H_{N,L}$ is given by the N-fold product of the one-particle ground state, the zero-momentum mode. His observation was called Bose-Einstein condensation, whence the ground state of $H_{N,L}$ became a Bose-Einstein condensate state. This is a state which is forbidden for fermions due to Pauli's exclusion principle. Ever since, people tried to generalize the definition of Bose-Einstein condensation and to prove analogous results for real, interacting gases. Nowadays, it is agreed to define Bose-Einstein condensation in terms of eigenvalues of one-particle density matrices[1], see [12, pp.4]. As opposed to the ideal gas, this definition includes the weakening that only a large fraction of the particles will condense. In general, given the interaction potential V, people are interested in studying questions of the type:

(Q1) Under which circumstances does Bose-Einstein condensation exist?

(Q2) Assuming Bose-Einstein condensation, what can we say about the ground state energy density (1.3) in the thermodynamic limit?

It turned out that addressing either of questions (Q1) or (Q2) for an interacting gas is severely more complicated than for the ideal gas. In fact, no systematic treatment of the Hamiltonian (1.1) was available whatsoever until 1947. In that year, the pioneering work [7] was published by N.N. Bogolubov. His paper introduced a procedure which intends to simplify $H_{N,L}$ from (1.1) in such a way that, afterwards, the ground state energy density (1.3) became computable. Nowadays, that procedure is called the Bogolubov approximation. Still, results on (Q1) remain unknown except for the very special case of hard sphere bosons [12, p.5]. Concerning (Q2), the method Bogolubov introduced was used in 1957 to derive an expansion of the ground state energy density (1.3) for a low-density, or dilute, gas [8]. Today, the formula is well known as the Lee-Huang-Yang formula after the authors T.D. Lee, K. Huang and C.N. Yang. It states that (1.3) is given by

$$e_0(\rho) = 4\pi a\rho\left[1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + \mathrm{o}(\rho a^3)^{1/2}\right] \qquad \text{as } \rho a^3 \to 0. \tag{1.4}$$

Here, a is the scattering length of the two-body interaction potential V and has the interpretation of an effective interaction range. We give a careful definition of a in Section 2. The term “dilute” refers to the assumption that the mean distance $\rho^{-1/3}$ of the particles is much bigger than a, i.e., $\rho^{1/3}a \ll 1$, or, equivalently, $\rho a^3 \ll 1$. This asymptotic expansion is really a series in the dimensionless[2] variable $0 \leqslant \rho^{1/3}a \ll 1$ and not only in the density ρ of the gas. See [12, p.167] for a detailed explanation.

Until the present day, mathematicians have tried to turn the methods of [7] and [8] into a mathematical proof of the formula (1.4). In fact, there is no rigorous understanding of the Lee-Huang-Yang formula to second order. The first-order term $4\pi\rho a$ is given by the ground state energy of the two-body problem, multiplied by the number of pairs in the gas. It was investigated for the first time by F.J. Dyson [9], who presented a rigorous upper and lower bound in 1957. He considered hard-core potentials and only the upper bound was matching (1.4). However, for more than 40 years, this was the best bound available. Dyson's method was generalized and improved by E. Lieb and J. Yngvason [10] for general potentials in 1998. Since then, the first-order term is known to match $4\pi a\rho$ in (1.4).

[1] For an introduction to the concept of one-particle, the interested reader is referred to [5, Chapter 8].
[2] See also [4, p.3].

1.3 Recent results

The experimental realization [11] of Bose-Einstein condensation in 1995 renewed the mathematical interest in proving rigorous results on the ground state energy of the Bose gas. In particular, understanding the second order term in (1.4) became of great interest, since this term is agreed to come from a quantum mechanical correlation effect [12, p.167]. We mention the work of L. Erdős, B. Schlein and H.-T. Yau [1] in 2008, who consider an interaction of the form λV, where $\lambda > 0$ is a tunable parameter and chosen to be small. In their paper, a trial state is constructed to prove that

$$e_0(\rho) \leqslant 4\pi a\rho\left[1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} S_\lambda\right] + \mathcal{O}(\rho^2|\ln\rho|) \qquad \text{as } \rho \to 0. \tag{1.5}$$

Here, S_λ is a specific constant satisfying $1 \leqslant S_\lambda \leqslant 1 + C\lambda$ for some $C > 0$, and a is the scattering length of λV. One sees that in the limit $\lambda \to 0$, the second order constant matches (1.4). Written in this form, the statement is unsatisfactory though, since, in fact, a depends on λ and goes to 0 with $\lambda \to 0$ in that limit as well. After all, the potential also scales down to 0. In Section 4, when more notation is available, we present a more detailed version of this statement, where this ambiguity does not occur. In 2009, a more complicated trial state was constructed by H.T. Yau and J. Yin [13]. It has an energy matching the second order term in (1.4). One crucial difference between these two trial states is that the one by Erdős et al. is so-called quasi-free as opposed to the one by Yau and Yin. The quasi-free states form a class of “simple” states. For a long time, it was believed that these states model the ground state energy density to second order. The paper [1] was the first hint that this might not be correct in general. In contrast, Yau and Yin proved that it is nevertheless possible to lower the energy to (1.4) if one increases the complexity of the chosen trial state. By giving a lower bound similar to (1.5), we prove that (1.4) is not reachable within the set of quasi-free states. The mathematical formulation of this statement is our main result, Theorem 1.3 below.

Let us briefly describe the origin of the functional, which we take into consideration for the proof of our main result. In a new two-component paper from 2015, J.P. Solovej, R. Reuvers, and M. Napiórkowski analyze the so-called Bogolubov free energy functional for temperatures $T \geqslant 0$. In the first paper [2], they provide existence results for minimizers. The second paper [3] contains

1. an existence result for a phase transition (Bose-Einstein condensation) and
2. a proof of an asymptotic energy expansion for the infimum of this functional for “moderate temperatures” and “low temperatures”.

These items are addressing the questions (Q1) and (Q2), respectively. As temperature is involved, the results look relatively complicated. In the present thesis, we simplify the asymptotic energy expansion [3, Theorem 10 (2)] in the special case $T = 0$, similar to (1.4), by using methods from [3]. Hence, we define our setup in a similar spirit to [3]. After having proved our main result, Theorem 1.3, we shall compare it to (1.5) in Section 4. In that spirit, this thesis is studying the question (Q2) from Subsection 1.2.

1.4 The functional

The canonical zero temperature Bogolubov energy functional is given by [3, p.3]

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) := (2\pi)^{-3}&\int_{\mathbb{R}^3} p^2\gamma(p)\,\mathrm{d}p + \frac{1}{2}\widehat{V}(0)\rho^2 \\ &+ (2\pi)^{-3}\rho_0\int_{\mathbb{R}^3}\widehat{V}(p)\left(\gamma(p)+\alpha(p)\right)\,\mathrm{d}p \\ &+ (2\pi)^{-6}\cdot\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\widehat{V}(p-q)\left(\gamma(p)\gamma(q)+\alpha(p)\alpha(q)\right)\,\mathrm{d}p\mathrm{d}q,\end{aligned} \tag{1.6}$$

where $\widehat{V}$ is the Fourier transform defined in (1.10) and ρ is given by (1.7) below. The functional $\mathcal{F}^{\mathrm{can}}$ is defined on the domain

$$\mathcal{D} := \{(\gamma,\alpha,\rho_0) : \gamma \in L^1((1+p^2)\mathrm{d}p),\ \gamma \geqslant 0,\ \alpha^2 \leqslant \gamma(\gamma+1),\ \rho_0 \geqslant 0\}.$$

$\mathcal{F}^{\mathrm{can}}$ describes a homogeneous, interacting Bose gas at temperature zero in 3 spatial dimensions in the thermodynamic limit. We make more precise what we mean by the term "homogeneous" in Remark 1.1. The pair (γ,α) models the one-particle density matrix of a quantum state. Here, γ is the momentum distribution of the gas and α is describing the long range correlations between the particles, which are assumed to be present in the ground state. The density $\rho_0 \geqslant 0$ of the condensate fraction is reflecting the macroscopic occupation of the one-particle ground state. Thus, the total density $\rho \geqslant 0$ is given by

$$\rho := \rho_0 + \rho_\gamma := \rho_0 + (2\pi)^{-3}\int_{\mathbb{R}^3}\gamma(p)\,\mathrm{d}p. \tag{1.7}$$

Remark 1.1 (Connection to (1.1))**.** Let us briefly discuss the connection of the functional $\mathcal{F}^{\mathrm{can}}$ in (1.6) with the Hamiltonian (1.1). A heuristic derivation of the functional can be found in Appendix A of [2]. To summarize, one starts with the N-body Hamiltonian $H_{N,L}$ in (1.1) with periodic boundary conditions. One evaluates the second quantized version of $H_{N,L}$ at a quantum state of finite particle expectation, whose one-particle density matrix $(\widetilde{\gamma},\widetilde{\alpha})$ is related to (γ,α). Since this remark cannot be turned into a mathematical statement (see below), we refrain from being more precise. Here, $\widetilde{\gamma}$ is a positive semi-definite trace-class operator on the one-particle Hilbert space $L^2(\Lambda)$ and $\widetilde{\alpha}$ satisfies[3]

$$\widetilde{\gamma} \geqslant \widetilde{\alpha}J(1+\widetilde{\gamma})^{-1}J\widetilde{\alpha}^*. \tag{1.8}$$

Furthermore, one makes use of the assumption that $(\widetilde{\gamma},\widetilde{\alpha})$ is translation invariant in the sense that the Fourier representations of the kernels of $\widetilde{\gamma}$ and $\widetilde{\alpha}$ are diagonal on $\frac{2\pi}{L}(\mathbb{Z}^3\times\mathbb{Z}^3)$, respectively. This is what we mean by the term "homogeneous" in the definition (1.6) above. With the additional assumption that α is real-valued, (1.8) becomes $\alpha^2 \leqslant \gamma(\gamma+1)$. Finally, one assumes that the quantum state is quasi-free which results in $\alpha^2 = \gamma(\gamma+1)$, see [5, Theorem 10.4]. Denoting the expected number of particles in the condensate by N_0, one can define the condensate density $\rho_0 := \frac{N_0}{L^3}$. Taking the informal limit $L \to \infty$, keeping the condensate density ρ_0 constant then yields (1.6). However, it is this limiting process which, to the best of the author's knowledge, makes a rigorous connection between $H_{N,L}$ and (1.6) unknown[4]. For clarity, we collect all assumptions on the states (γ,α) which we used on the way:

[3]See, for example, [14, Lemma 1.1]. The map J is the Hilbert space identification $L^2(\Lambda) \to L^2(\Lambda)^*$ – in our case the complex conjugation.

[4]We refer to the remark "up to technical details involving the thermodynamic limit" on [3, p.4].

(1) α is real valued,

(2) $(\widetilde{\gamma}, \widetilde{\alpha})$ is quasi-free,

(3) $(\widetilde{\gamma}, \widetilde{\alpha})$ is translation invariant.

We conclude the remark by noting that, due to the limit $L \to \infty$ instead of $N = \rho L^3 \to \infty$, the Lee-Huang-Yang formula (1.4) becomes

$$e_0(\rho)\rho = 4\pi a\rho^2 + \frac{512\sqrt{\pi}}{15}(\rho a)^{5/2} + \mathrm{o}(\rho a)^{5/2} \qquad \text{as } \rho a \to 0. \tag{1.9}$$

1.5 Assumptions on the potential

In our model, the particles interact through a repulsive and real-valued two-body potential $V\colon \mathbb{R}^3 \to \mathbb{R}$. In the following, we shall fix the assumptions which we put on V.

Assumption 1.2. Let $V\colon \mathbb{R}^3 \to \mathbb{R}$ be a measurable potential and assume that the following statements hold:

(1) $V \in L^1(\mathbb{R}^3)$ and the Fourier transform satisfies $\widehat{V} \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$.

(2) V is radially symmetric, meaning that $V(Rx) = V(x)$ for every $R \in \mathrm{SO}(3)$, $x \in \mathbb{R}^3$. Here, $\mathrm{SO}(3)$ is the set of special orthogonal matrices $R \in \mathbb{R}^{3\times 3}$ with $RR^t = \mathbb{1}$ and $\det R = 1$.

(3) V and $\widehat{V}$ are nonnegative on $\mathbb{R}^3$ and $\widehat{V}(0) > 0$. Furthermore, V has compact support, i.e., there is $R_0 > 0$ such that $V \equiv 0$ on $B_{R_0}(0)^c \subseteq \mathbb{R}^3$. Here, $B_R(0)$ is the ball in $\mathbb{R}^3$ of radius $R > 0$, centered about the origin.

(4) $\widehat{V} \in C^1(\mathbb{R}^3)$, i.e., $\widehat{V}$ is continuously differentiable on $\mathbb{R}^3$.

We use the convention that the Fourier transform $\widehat{V}$ of V is denoted by

$$\widehat{V}(p) := \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}px} V(x)\,\mathrm{d}x. \tag{1.10}$$

Let us collect some properties that follow from Assumption 1.2. From (2) we have that $V(-x) = V(x)$ for all $x \in \mathbb{R}^3$ by choosing a special orthogonal matrix that rotates around an axis perpendicular to x. Moreover, for $R \in \mathrm{SO}(3)$ and $p \in \mathbb{R}^3$, we get

$$\widehat{V}(Rp) = \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}pR^{-1}x} V(x)\,\mathrm{d}x = \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}px} V(Rx) = \widehat{V}(p).$$

By similar arguments as for V, we get $\widehat{V}(p) = \widehat{V}(-p) = \overline{\widehat{V}(p)}$, so that $\widehat{V}$ is real valued and symmetric. Therefore, the assumption that $\widehat{V} \geqslant 0$ makes sense. Furthermore, $\widehat{V}(0) > 0$ implies that $V \not\equiv 0$. We expect that the last assumption (4) can be relaxed to Lipschitz continuity at 0 but for simplicity, we work with (4).

1.6 Main result

The canonical minimization problem for $\mathcal{F}^{\mathrm{can}}$ reads [3, p.3]

$$F(\rho) := \inf_{\substack{(\gamma,\alpha,\rho_0)\in\mathcal{D} \\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) = \inf\{f(\rho, \rho_0) : 0 \leqslant \rho_0 \leqslant \rho\}, \tag{1.11}$$

where

$$f(\rho, \rho_0) = \inf\{\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) : (\gamma, \alpha, \rho_0) \in \mathcal{D},\ \rho_0 = \rho - \rho_\gamma\}.$$

In that sense, the condition $\rho_\gamma = \rho - \rho_0$, given in (1.7), can be understood as a constraint to which the minimization problem (1.11) for $\mathcal{F}^{\mathrm{can}}$ is subject. We have to take it into account throughout the thesis. Our main result reads as follows.

Theorem 1.3. *Let V be a potential satisfying Assumption 1.2. Let $a > 0$ denote its scattering length as defined in Definition 2.1 and define the quantity*

$$\nu := \frac{\widehat{V}(0)}{8\pi a}. \tag{1.12}$$

Assume that

$$1 < \nu < \frac{3}{2}. \tag{1.13}$$

Then, for $\rho \geqslant 0$, the canonical minimization problem $F(\rho)$ in (1.11) admits the following asymptotic expansion as $\rho a \to 0$:

$$F(\rho) = 4\pi a \rho^2 + (8\pi)^{5/2} \cdot I(2\nu - 1) \cdot (\rho a)^{5/2} + \mathrm{o}(\rho a)^{5/2}, \tag{1.14}$$

where, for $\sigma \in [1, \infty)$,

$$I(\sigma) := (2\pi)^{-3} \cdot \frac{1}{2} \int_{\mathbb{R}^3} \left\{ \sqrt{p^4 + 2\sigma p^2 + \sigma^2 - 1} - p^2 - \sigma + \frac{1}{2p^2} \right\} \mathrm{d}p. \tag{1.15}$$

It is a known fact that $\widehat{V}(0) \geqslant 8\pi a$, see [12, eq.(C.10)]. Hence, it is clear from the definition (1.12) that $\nu \geqslant 1$. The assumption that additionally $\nu > 1$ holds is essential for our proof, whereas $\nu < 3/2$ is only assumed for technical reasons and can be relaxed. However, we are interested in $1 < \nu \ll 3/2$ anyway. We are going to prove that I in (1.15) is strictly monotonically increasing on $[1, \infty)$ and, furthermore, that $I(1) = \frac{2\sqrt{2}}{15\pi^2}$. Hence,

$$(8\pi)^{5/2} I(1) = 8^2 \pi^2 \cdot 2\sqrt{2\pi} \cdot \frac{2\sqrt{2}}{15\pi^2} = \frac{512\sqrt{\pi}}{15}.$$

This is precisely the constant in front of the second order term in the Lee-Huang-Yang formula, i.e., in the limit $\nu \to 1$, we recover (1.9). For a homogeneous gas, this proves that, within the quasi-free translation invariant states, the infimum as it is stated in (1.9) cannot be reached.

1.7 Plan for the thesis

In Section 2, we consider the two-body problem given by the potential V. We define the scattering length a and the scattering solution u of the potential $\widehat{V}$ properly. The scattering solution satisfies the differential equation

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

in $\mathbb{R}^3$ with $u(x) \to 1$ as $|x| \to \infty$. Here, we borrow the existence and uniqueness result [4, Theorem 1.2.2], which includes a complete proof. From this, we derive several integral equations involving u and V and conclude a representation of the scattering equation in momentum space. This preparation will be useful for Section 3, where we prove Theorem 1.3. For this purpose, we define a simplified functional which does not depend on α anymore. The simplified functional serves as a lower bound to $\mathcal{F}^{\text{can}}$ and its ground state γ_{min} can be computed explicitly. Afterwards, we need to approximate the ground state energy of the simplified functional to the appropriate precision for (1.14). We make use of an a priori estimate which states that $\rho - \rho_0 = \mathcal{O}(\rho)^{3/2}$, i.e., ρ_0 is "almost all of" ρ. This gives the lower bound. For the upper bound, the state γ_{min} – together with some suitably chosen α_{min} – is the candidate for a trial state which we insert into $\mathcal{F}^{\text{can}}$. We need to compute the energy and estimate the error terms. The concluding Section 4 consists of a comparison of our low-density expansion with the energy of the trial state in [1]. It turns out that the energy is (1.14) to second order. In view of the paper [13], we point out possible extensions of Theorem 1.3.

2 The Scattering Length

2.1 Definition and elementary properties

In this section, we define the scattering length a of the potential V. In the first step, we present the existence result [4, Theorem 1.2.2] for the scattering solution u in Theorem 2.2. Afterwards, we use the result to prove that $1-u$ may be Fourier transformed in the sense of $\mathcal{S}'(\mathbb{R}^3)$. On the way, we collect several integral equations involving u and the potential V. Here, we make partial use of [3, p.11]. The conclusion is a Plancherel-type equality for V and $1-u$. The preparation of this section will be useful for the main section, Section 3, where we prove Theorem 1.3.

Definition 2.1. Let $V\colon \mathbb{R}^3 \to \mathbb{R}$ be a nonnegative, radially symmetric and measurable potential. The scattering length a of V is defined by

$$a := \frac{1}{8\pi} \cdot \inf_u \left(\int_{\mathbb{R}^3} |\nabla u|^2 + \frac{1}{2} \int_{\mathbb{R}^3} V|u|^2 \right), \tag{2.1}$$

where the infimum is taken over all nonnegative, radially symmetric functions $u \in H^1_{\mathrm{loc}}(\mathbb{R}^3)$ with[5] $u(x) \to 1$ as $|x| \to \infty$. If the infimum is attained for such a function u, we call u a scattering solution of V.

From the condition $V \geqslant 0$ it follows immediately that $a \geqslant 0$.

Theorem 2.2 [4, Theorem 1.2.2]**.** *Let $V \in L^1(\mathbb{R}^3)$ be a nonnegative, radially symmetric and compactly supported potential. Then, the infimum* (2.1) *is attained for a unique function $u \in H^1_{\mathrm{loc}}(\mathbb{R}^3)$ such that*

(a) u satisfies the scattering equation

$$-\Delta u + \frac{1}{2} V u = 0 \tag{2.2}$$

in the sense of distributions $\mathcal{S}'(\mathbb{R}^3)$.

(b) Moreover, u is continuous, radially symmetric, and radially increasing.

(c) With $a \geqslant 0$ as in Definition 2.1*, we have*

$$u(x) \geqslant 1 - \frac{a}{|x|}, \tag{2.3}$$

with equality for $|x| \geqslant R_0$, where $R_0 > 0$ is such that $V \equiv 0$ on $B_{R_0}(0)$.

(d) In particular, $0 \leqslant u < 1$ holds.

(e) If additionally $V \not\equiv 0$, then we have that $a > 0$.

Since V satisfies Assumption 1.2, Theorem 2.2 applies and provides a scattering solution u. Define the function

$$g(x) := V(x)u(x) = V(x)(1 - w(x))$$

[5] Radially symmetric functions $u \in H^1_{\mathrm{loc}}(\mathbb{R}^3)$ are continuous away from the origin, see [4, p.9]. Therefore, this convergence is to be understood pointwise.

and, for $x \in \mathbb{R}^3$, consider

$$\Gamma(g)(x) := \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{g(y)}{|x-y|} \, \mathrm{d}y.$$

For $x \in B_{R_0}(0)^c$, i.e., $x \notin \operatorname{supp}(g) \subseteq \operatorname{supp}(V)$, we have

$$|\Gamma(g)(x)| \leqslant \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{|g(y)|}{|x-y|} \, \mathrm{d}y \leqslant \frac{1}{4\pi} \frac{\|g\|_{L^1(\mathbb{R}^3)}}{\operatorname{dist}(x, \operatorname{supp}(g))} \xrightarrow{|x| \to \infty} 0, \tag{2.4}$$

so that $\Gamma(g)$ is a bounded function on $\mathbb{R}^3$. A mollification argument for g shows that

$$- \int_{\mathbb{R}^3} \Gamma(g) \cdot \Delta \varphi = \int_{\mathbb{R}^3} g \cdot \varphi$$

for every test function $\varphi \in \mathcal{S}(\mathbb{R}^3)$. On the other hand, define $w := 1 - u$ and note that $0 \leqslant w \leqslant 1$ by Theorem 2.2 (d). Furthermore, $w(x) \to 0$ as $|x| \to \infty$. Note that by Assumption 1.2 (1), V is continuous and thus, g is continuous since, by Theorem 2.2 (b), u is. By Theorem 2.2 (a), we infer that $w - \frac{\Gamma(g)}{2}$ is a bounded harmonic function on $\mathbb{R}^3$. Hence, it is constant by Liouville's theorem. Since $\Gamma(g)$ goes to zero at infinity by (2.4), we conclude that this constant is zero and hence $w(x) = \frac{1}{2}\Gamma(g)(x)$ for each $x \in \mathbb{R}^3$. For $|x| > R_0$ we also have that $w(x) = \frac{a}{|x|}$ by Theorem 2.2 and thus, for such x, we get

$$w(x) = \frac{a}{|x|} = \frac{1}{8\pi} \int_{\mathbb{R}^3} \frac{g(y)}{|x-y|} \, \mathrm{d}y.$$

Hence, for $|x| > R_0$, we obtain

$$8\pi a = \int_{\mathbb{R}^3} \frac{|x|}{|x-y|} \cdot g(y) \, \mathrm{d}y \xrightarrow{|x| \to \infty} \int_{\mathbb{R}^3} g(y) \, \mathrm{d}y$$

by the dominated convergence theorem. The dominant is given by $\frac{|x|}{\operatorname{dist}(x, \operatorname{supp} g)} g(y) \leqslant g(y)$. By the definition of the Fourier transform, we arrive at the first representation of the scattering length as

$$8\pi a = \widehat{g}(0) = \widehat{Vu}(0). \tag{2.5}$$

In comparison, we define the first order Born approximation a_0 of the potential V as

$$8\pi a_0 := \widehat{V}(0),$$

see also [4, p.5]. It is known that $a_0 \geqslant a$ (see equation (C.10) in [12]). Motivated by this, we consider the parameter $\nu = \frac{a_0}{a} \geqslant 1$ as in (1.12) in our main theorem. According to (1.13), we assume that even strict inequality holds, i.e., $\nu > 1$. It is not clear to the author whether this holds in general but it is claimed in [1, eq.(8)] and [3, p.4]. The arguments there seem not to be sufficient for that conclusion. However, an important insight is given by the proof of [4, Theorem 1.2.2]. In point 5, the author proves that $a > 0$ unless $V \equiv 0$, our assertion (e) of Theorem 2.2. The proof uses the scattering equation and the fact that u is subharmonic due to $V \geqslant 0$. Therefore, it is convincing to apply the same strategy to prove that $a_0 - a > 0$. That, in turn, would imply that $\nu > 1$. Presumably, one needs to apply elliptic regularity methods in advance so that we are not going to pursue this idea further here. As mentioned in the introduction, the additional assumption that $\nu < 3/2$ holds is only for technical reasons and not necessary. One can easily generalize the corresponding proofs for $\nu \geqslant 3/2$.

2.2 A Fourier representation of the scattering solution

Recall that w is a bounded continuous function and $Vu \in L^1(\mathbb{R}^3)$. Hence, w and Vu belong to the space $\mathcal{S}'(\mathbb{R}^3)$ of tempered distributions and by the scattering equation, we have

$$0 = \int_{\mathbb{R}^3} w \cdot \Delta\varphi + \frac{1}{2}\int_{\mathbb{R}^3} Vu \cdot \varphi$$

for every $\varphi \in \mathcal{S}(\mathbb{R}^3)$, the Schwartz space on $\mathbb{R}^3$. Hence, denoting the Fourier transform by $\mathcal{F}\colon \mathcal{S}' \to \mathcal{S}'$, we have

$$\frac{1}{2}\int_{\mathbb{R}^3} \widehat{Vu} \cdot \varphi = \frac{1}{2}\int_{\mathbb{R}^3} Vu \cdot \widehat{\varphi} = -\int_{\mathbb{R}^3} w \cdot \Delta\widehat{\varphi} = \int_{\mathbb{R}^3} w \cdot \widehat{p^2\varphi} = \mathcal{F}(w)(p^2\varphi)$$

so that, by replacing $p^2\varphi \in \mathcal{S}(\mathbb{R}^3)$ with $\varphi \in \mathcal{S}(\mathbb{R}^3)$, we get

$$\int_{\mathbb{R}^3} w(x) \cdot \widehat{\varphi}(x)\,\mathrm{d}x = \mathcal{F}(w)(\varphi) = \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)}{2p^2} \cdot \varphi(p)\,\mathrm{d}p \tag{2.6}$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^3)$. We want to extend (2.6) to $\widehat{Vu}$. To do this, we choose a sequence $(\varphi_n)_n \subseteq \mathcal{S}(\mathbb{R}^3)$ of radially symmetric functions $\varphi_n \in \mathcal{S}(\mathbb{R}^3)$ so that $\varphi_n \to \widehat{Vu}$ in $L^1(\mathbb{R}^3)$ as $n \to \infty$. Note that, since $w \in L^\infty(\mathbb{R}^3)$, and since Vu is radially symmetric, the convergence of the left-hand side of (2.6) is automatically

$$\int_{\mathbb{R}^3} w(x)\widehat{\varphi}_n(x)\,\mathrm{d}x \xrightarrow{n\to\infty} (2\pi)^3 \int_{\mathbb{R}^3} w(x)Vu(x)\,\mathrm{d}x.$$

On the other hand,

$$\int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)}{p^2} \cdot \left[\varphi_n(p) - \widehat{Vu}(p)\right]\mathrm{d}p = 4\pi \int_0^\infty \widehat{Vu}(r) \cdot \left[\varphi_n(r) - \widehat{Vu}(r)\right]\mathrm{d}r$$

and, since $\widehat{Vu}$ is bounded and continuous as well, we get the convergence of the right-hand side of (2.6). To summarize, we obtain

$$\int_{\mathbb{R}^3} w(x) \cdot Vu(x)\,\mathrm{d}x = (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)^2}{2p^2}\,\mathrm{d}p < \infty. \tag{2.7}$$

Motivated by (2.6), we define, in slight abuse of notation,

$$\widehat{w}(p) := \frac{\widehat{Vu}(p)}{2p^2}. \tag{2.8}$$

In Section 3, we need $\widehat{w}$ to be more regular. Therefore, we prove some regularity estimates in the next subsection.

2.3 Regularity estimates for the scattering solution

We mainly imitate [3, p.11] and start by noting that $Vu \geqslant 0$ since $u \geqslant 0$, see Theorem 2.2 (d). From this, we get

$$|\widehat{V}(p)| \leqslant \widehat{V}(0) = 8\pi a_0 = 8\pi a \cdot \nu, \qquad |\widehat{Vu}(p)| \leqslant \widehat{Vu}(0) = 8\pi a. \tag{2.9}$$

From (2.7), we get

$$\int_{\mathbb{R}^3} V(x)u(x)^2 \,\mathrm{d}x = 8\pi a - \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)^2}{2p^2} \,\mathrm{d}p < \infty.$$

By a similar approximation argument to (2.7), we obtain that

$$(2\pi)^{-3} \int_{\mathbb{R}^3} |\widehat{Vu}(p)|^2 \,\mathrm{d}p = \int_{\mathbb{R}^3} |Vu(x)|^2 \,\mathrm{d}x \leqslant \|V\|_\infty \int_{\mathbb{R}^3} V(x)u(x)^2 \,\mathrm{d}x < \infty.$$

With this, we may estimate further

$$\begin{aligned}\left\| \frac{\widehat{Vu}}{p^2} \right\|_{L^1(\mathbb{R}^3)} &\leqslant \int_{|p|\leqslant 1} \frac{|\widehat{Vu}(p)|}{p^2} \,\mathrm{d}p + \int_{|p|\geqslant 1} \frac{|\widehat{Vu}(p)|}{p^2} \,\mathrm{d}p \\ &\leqslant 4\pi \widehat{Vu}(0) + \left(\int_{|p|\geqslant 1} |\widehat{Vu}(p)|^2 \,\mathrm{d}p \right)^{1/2} \left(\int_{|p|\geqslant 1} \frac{1}{p^4} \,\mathrm{d}p \right)^{1/2} < \infty.\end{aligned}$$

Note that, by definition (2.8), this means

$$\widehat{w} \in L^1(\mathbb{R}^3). \tag{2.10}$$

Now, let $\varphi \in \mathcal{S}(\mathbb{R}^3)$ and note that

$$\widehat{\widehat{V} * \varphi} = (2\pi)^3 \cdot V \cdot \widehat{\varphi}$$

as L^1-functions. Going back to (2.6), we can insert $\widehat{V} * \varphi \in \mathcal{S}(\mathbb{R}^3)$. We get

$$\int_{\mathbb{R}^3} w(x)V(x)\widehat{\varphi}(x) \,\mathrm{d}x = (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)}{2p^2} \cdot (\widehat{V} * \varphi)(p) \,\mathrm{d}p. \tag{2.11}$$

Choose a sequence $(\varphi_n)_n \in \mathcal{S}(\mathbb{R}^3)$ with $\|\widehat{\varphi}_n - 1\|_\infty \to 0$ as $n \to \infty$. Since $Vw \in L^1(\mathbb{R}^3)$, we conclude that the left-hand side of (2.11) converges to $\widehat{Vw}(0)$. Using (2.10) and the continuity of the Fourier transform, we finally infer that (2.11) converges to the Plancherel-type equality

$$\int_{\mathbb{R}^3} V(x)w(x) \,\mathrm{d}x = (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)}{2p^2} \cdot \widehat{V}(p) \,\mathrm{d}p = (2\pi)^{-3} \int_{\mathbb{R}^3} \widehat{w}(p) \cdot \widehat{V}(p) \,\mathrm{d}p. \tag{2.12}$$

We conclude this section by noting that

$$\widehat{Vw} = \widehat{w} * \widehat{V} \in L^1(\mathbb{R}^3), \tag{2.13}$$

since both function belong to $L^1(\mathbb{R}^3)$, see (2.10).

3 Minimization of the Functional

In this section, we prove the main result, Theorem 1.3. The first thing to do is to prove that the functional $\mathcal{F}^{\text{can}}$ is well-defined on its domain. This is the starting point. By making use of the scattering equation (2.8), we define a simplified functional $\mathcal{F}^{\text{sim}}$ afterwards. The simplified functional will serve as a lower bound for $\mathcal{F}^{\text{can}}$ and can be minimized explicitly. We have to spend some time on proving that, indeed, the minimizer is an allowed trial function. We do this simultaneously with proving the approximations of the occuring integrals to the required precision. When we have this, we can start to consider lower and upper bounds to prove the claimed asymptotics (1.14) for the canonical minimization problem (1.11). Of course, the minimizer of $\mathcal{F}^{\text{sim}}$ serves as a test function for the upper bound for $\mathcal{F}^{\text{can}}$. There are error terms which have to be estimated.

Recall from (1.6) that the full functional is given by

$$\begin{aligned}\mathcal{F}^{\text{can}}(\gamma,\alpha,\rho_0) = (2\pi)^{-3}\int_{\mathbb{R}^3} p^2\gamma(p)\,\mathrm{d}p + \frac{1}{2}\widehat{V}(0)\rho^2 \\ + (2\pi)^{-3}\rho_0\int_{\mathbb{R}^3}\widehat{V}(p)(\gamma(p)+\alpha(p))\,\mathrm{d}p + Q(\gamma,\gamma) + Q(\alpha,\alpha),\end{aligned} \tag{3.1}$$

where the symmetric quadratic form Q is defined as

$$Q(\varphi,\psi) := (2\pi)^{-6}\cdot\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\widehat{V}(p-q)\varphi(p)\psi(q)\,\mathrm{d}p\mathrm{d}q. \tag{3.2}$$

The functional $\mathcal{F}^{\text{can}}$ is defined on the domain

$$\mathcal{D} = \{(\gamma,\alpha,\rho_0) : \gamma\in L^1((1+p^2)\mathrm{d}p),\ \gamma\geqslant 0,\ \alpha^2\leqslant\gamma(\gamma+1),\ \rho_0\geqslant 0\} \tag{3.3}$$

and, according to (1.7), the densities $\rho,\rho_0\geqslant 0$ satisfy the contraint

$$\rho = \rho_0 + \rho_\gamma = \rho_0 + (2\pi)^{-3}\int_{\mathbb{R}^3}\gamma(p)\,\mathrm{d}p. \tag{3.4}$$

3.1 Well-definedness of the functional

We use Assumption 1.2 on the potential V to prove that $\mathcal{F}^{\text{can}}$ is well-defined on $\mathcal{D}$. We proceed as in [2, p.11]. Fix $(\gamma,\alpha,\rho_0)\in\mathcal{D}$ and decompose α according to $\alpha = \alpha_> + \alpha_<$, where $\alpha_> := \alpha\cdot\mathbb{1}_{\{\gamma\geqslant 1\}}$ and $\alpha_< := \alpha\cdot\mathbb{1}_{\{\gamma<1\}}$. Then,

$$|\alpha_<| \leqslant \sqrt{\gamma^2+\gamma}\cdot\mathbb{1}_{\{\gamma<1\}} \leqslant \sqrt{\gamma+\gamma}\cdot\mathbb{1}_{\{\gamma<1\}} \leqslant \sqrt{2}\cdot\sqrt{\gamma}\cdot\mathbb{1}_{\{\gamma<1\}}. \tag{3.5}$$

$$|\alpha_>| \leqslant \sqrt{\gamma^2+\gamma}\cdot\mathbb{1}_{\{\gamma\geqslant 1\}} \leqslant \sqrt{\gamma^2+\gamma^2} = \sqrt{2}\cdot\gamma. \tag{3.6}$$

We use this decomposition to estimate all the terms in (3.1). We start with the linear term for α and estimate

$$\begin{aligned}\int_{\mathbb{R}^3}\widehat{V}(p)\alpha(p)\,\mathrm{d}p &\leqslant \sqrt{2}\int_{\{\gamma<1\}}\widehat{V}(p)\sqrt{\gamma(p)}\,\mathrm{d}p + \sqrt{2}\int_{\{\gamma\geqslant 1\}}\widehat{V}(p)\gamma(p)\,\mathrm{d}p \\ &\leqslant \sqrt{2}\cdot\|\widehat{V}\|_{L^1(\mathbb{R}^3)} + \sqrt{2}\cdot\widehat{V}(0)\|\gamma\|_{L^1(\mathbb{R}^3)}.\end{aligned} \tag{3.7}$$

The linear term for γ is bounded by

$$\int_{\mathbb{R}^3}\widehat{V}(p)\gamma(p)\,\mathrm{d}p \leqslant \widehat{V}(0)\|\gamma\|_{L^1(\mathbb{R}^3)}, \tag{3.8}$$

and, in a similar fashion, we estimate

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \widehat{V}(p-q)\gamma(p)\gamma(q)\,\mathrm{d}p\mathrm{d}q \leqslant \widehat{V}(0)\|\gamma\|^2_{L^1(\mathbb{R}^3)}. \tag{3.9}$$

The estimate for $Q(\alpha,\alpha)$ in (3.1) is slightly more involved. Let us start by noting that

$$\begin{aligned}\alpha(p)\alpha(q) &= \alpha_>(p)\alpha_>(q) + \alpha_>(p)\alpha_<(q) + \alpha_<(p)\alpha_>(q) + \alpha_<(p)\alpha_<(q)\\ &\leqslant 2\gamma(p)\gamma(q) + 2\gamma(p) + 2\gamma(q) + 2\sqrt{\gamma(p)\gamma(q)}\\ &\leqslant 2\gamma(p)\gamma(q) + 2\gamma(p) + 2\gamma(q) + \sqrt{2}(\gamma(p)+\gamma(q)).\end{aligned}$$

With this, we can estimate

$$\begin{aligned}&\iint_{\mathbb{R}^3\times\mathbb{R}^3} \widehat{V}(p-q)\alpha(p)\alpha(q)\,\mathrm{d}p\mathrm{d}q \leqslant\\ &\qquad\leqslant 2\iint_{\mathbb{R}^3\times\mathbb{R}^3} \widehat{V}(p-q)\left[\gamma(p)\gamma(q) + 2\gamma(p) + \frac{1}{\sqrt{2}}(\gamma(p)+\gamma(q))\right]\mathrm{d}p\mathrm{d}q\\ &\qquad\leqslant 2\widehat{V}(0)\|\gamma\|^2_{L^1(\mathbb{R}^3)} + 2(2+\sqrt{2})\cdot\|\widehat{V}\|_{L^1(\mathbb{R}^3)}\cdot\|\gamma\|_{L^1(\mathbb{R}^3)}.\end{aligned} \tag{3.10}$$

This proves that all the terms in (3.1) are well-defined on $\mathcal{D}$. Let $Q(\varphi) := Q(\varphi,\varphi)$. We continue by remarking that if $\varphi \in L^1(\mathbb{R}^3)$, then

$$Q(\varphi) = (2\pi)^3\int_{\mathbb{R}^3}(\widehat{V}*\varphi)(p)\varphi(p)\,\mathrm{d}p = \int_{\mathbb{R}^3} V(x)|\check{\varphi}(x)|^2\,\mathrm{d}x \geqslant 0, \tag{3.11}$$

where $\check{\varphi} := \widehat{\varphi(-\cdot)}$. Hence, $Q(\gamma)\geqslant 0$. To arrive at the same statement for α, we borrow Young's inequality [15, Theorem 4.2].

Theorem 3.1 (Young's inequality). *Let $p,q,r \geqslant 1$ and $1/p + 1/q + 1/r = 2$. Let $f \in L^p(\mathbb{R}^3)$, $g \in L^q(\mathbb{R}^3)$ and $h \in L^r(\mathbb{R}^3)$. Then*

$$\left|\int_{\mathbb{R}^3}(f*g)(x)h(x)\,\mathrm{d}x\right| \leqslant C_{\mathrm{Y}}(p,q,r)\cdot\|f\|_{L^p(\mathbb{R}^3)}\|g\|_{L^q(\mathbb{R}^3)}\|h\|_{L^r(\mathbb{R}^3)}.$$

From (3.5) and (3.6), we infer that $\alpha_> \in L^1(\mathbb{R}^3)$ and $\alpha_< \in L^2(\mathbb{R}^3)$. Let $(\varphi_n)_n \subseteq \mathcal{S}(\mathbb{R}^3)$ be such that $\|\alpha_< - \varphi_n\|_2 \to 0$ as $n\to\infty$ and write

$$\alpha = \alpha_> + \varphi_n + (\alpha_< - \varphi_n). \tag{3.12}$$

Then, a straightforward computation shows that

$$Q(\alpha) = Q(\alpha_> + \varphi_n) + Q(\alpha_< - \varphi_n) + 2\cdot Q(\alpha_>, \alpha_< - \varphi_n) + 2\cdot Q(\varphi_n, \alpha_< - \varphi_n).$$

We have that $Q(\alpha_> + \varphi_n) \geqslant 0$ for all $n\in\mathbb{N}$ since $\alpha_> + \varphi_n \in L^1(\mathbb{R}^3)$. Due to Assumption 1.2 (1), we have that $\widehat{V} \in L^2(\mathbb{R}^3)$ and thus, applying Theorem 3.1 three times, we obtain

$$\begin{aligned}Q(\alpha) \geqslant -C_{\mathrm{Y},1}\|\widehat{V}\|_{L^1}\|\alpha_< - \varphi_n\|^2_{L^2} &- 2C_{\mathrm{Y},2}\cdot\|\widehat{V}\|_{L^2}\|\alpha_>\|_{L^1}\|\alpha_< - \varphi_n\|_{L^2}\\ &- 2C_{\mathrm{Y},3}\cdot\|\widehat{V}\|_{L^1}\|\varphi_n\|_{L^2}\|\alpha_< - \varphi_n\|_{L^2}.\end{aligned}$$

The right hand side converges to 0 as $n\to\infty$ and thus

$$Q(\alpha) \geqslant 0. \tag{3.13}$$

3.2 Simplified functional and errors

Now, we define the simplified functional $\mathcal{F}^{\text{sim}}$ and prove that, provided the error terms are small, $\mathcal{F}^{\text{sim}}$ may be equivalently minimized in place of $\mathcal{F}^{\text{can}}$. Set

$$\mathcal{D}^{\text{sim}} := \{(\gamma, \rho_0) : \gamma \in L^1((1+p^2)\mathrm{d}p),\ \gamma \geqslant 0,\ \rho_0 \geqslant 0\}. \tag{3.14}$$

Note that if $(\gamma, \alpha, \rho_0) \in \mathcal{D}$ as in (3.3) then $(\gamma, \rho_0) \in \mathcal{D}^{\text{sim}}$. For $(\gamma, \rho_0) \in \mathcal{D}^{\text{sim}}$ define

$$\begin{aligned}\mathcal{F}^{\text{sim}}(\gamma, \rho_0) := 4\pi a\rho^2 + 4\pi(a_0 - a)(\rho^2 - \rho_0^2) + (2\pi)^{-3} &\int_{\mathbb{R}^3} [p^2 + \rho_0 \widehat{V}(p)]\gamma(p)\,\mathrm{d}p \\ - (2\pi)^{-3}\rho_0 &\int_{\mathbb{R}^3} |\widehat{Vu}(p)|\sqrt{\gamma(p)(\gamma(p)+1)}\,\mathrm{d}p \\ + (2\pi)^{-3}\frac{\rho_0^2}{2} &\int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)^2}{2p^2}\,\mathrm{d}p.\end{aligned} \tag{3.15}$$

By (2.13), we have that $\widehat{Vu} \in L^1(\mathbb{R}^3)$ and thus the finiteness of the second line follows from (3.7) together with the same split $\gamma \geqslant 1$ and $\gamma \leqslant 1$ as in (3.5) and (3.6). The third line is finite because of (2.7).

Note that $\mathcal{F}^{\text{sim}}$ is considerably simpler than $\mathcal{F}^{\text{can}}$ since it does not depend on α anymore and it is linear in γ aside from the term with the square root. Moreover, the desired first order term $4\pi a\rho^2$ in (1.14) appears directly in front. Of course, this is a little bit artificial since it is also contained in the second term. However, by assumption[6], most of the particles are in the condensate state which, in turn, means that ρ_0 is "almost all of ρ". That statement is quantified as $\rho - \rho_0 = \mathcal{O}(\rho)^{3/2}$ in Lemma 3.15 below. As a consequence, $\rho^2 - \rho_0^2$ is small compared to ρ^2. When we compare $\mathcal{F}^{\text{can}}$ and $\mathcal{F}^{\text{sim}}$, error terms are going to arise. Let us summarize them in the following lines:

$$E_1(\gamma, \alpha, \rho_0) := (2\pi)^{-3} \cdot \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \widehat{V}(p-q)\gamma(p)\gamma(q)\,\mathrm{d}p\mathrm{d}q, \tag{3.16}$$

$$E_2(\gamma, \alpha, \rho_0) := (2\pi)^{-3} \cdot \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \widehat{V}(p-q)(\alpha(p) + \rho_0\widehat{w}(p))(\alpha(q) + \rho_0\widehat{w}(q))\,\mathrm{d}p\mathrm{d}q, \tag{3.17}$$

$$E_3(\gamma, \alpha, \rho_0) := (2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} \widehat{Vu}(p)\alpha(p) + |\widehat{Vu}(p)|\sqrt{\gamma(p)(\gamma(p)+1)}\,\mathrm{d}p, \tag{3.18}$$

where $\widehat{w}$ is as in (2.8). The first lemma states that minimizing the full functional and the simplified functional are equivalent provided the error terms are small.

Lemma 3.2. *Let $(\gamma, \alpha, \rho_0) \in \mathcal{D}$ and let $\mathcal{F}^{\text{sim}}(\gamma, \rho_0)$ be defined as in* (3.15)*. Let the error terms E_1, E_2 and E_3 be given as in* (3.16), (3.17) *and* (3.18)*, respectively. Then*

$$0 \leqslant \mathcal{F}^{\text{can}}(\gamma, \alpha, \rho_0) - \mathcal{F}^{\text{sim}}(\gamma, \rho_0) = (E_1 + E_2 + E_3)(\gamma, \alpha, \rho_0)$$

Proof. Recall that the scattering equation (2.8) reads $\widehat{w} = \frac{\widehat{Vu}}{2p^2}$ and that $\widehat{w} \in L^1(\mathbb{R}^3)$ due to (2.10). We compare[7] the function α with $-\rho_0\widehat{w}$. This leads to

$$Q(\alpha) = Q(\alpha + \rho_0\widehat{w}) - 2\rho_0 Q(\alpha, \widehat{w}) - \rho_0^2 Q(\widehat{w}). \tag{3.19}$$

[6]Compare question (Q2) in Subsection 1.2.

[7]For a heuristic reasoning, see Remark 3.3.

Note that, since $\widehat{w} \in L^1(\mathbb{R}^3)$, we have $Q(\widehat{w}) \geqslant 0$ because of (3.11) and $Q(\widehat{w}) < \infty$ by (3.9). Moreover,

$$Q(\alpha, \widehat{w}) = (2\pi)^{-3} \cdot \frac{1}{2} \int_{\mathbb{R}^3} \widehat{Vw}(p)\alpha(p)\,\mathrm{d}p. \tag{3.20}$$

By (2.13), we have $\widehat{Vw} \in L^1(\mathbb{R}^3)$ and thus $Q(\alpha, \widehat{w})$ is finite by (3.7). Finally, note that $\alpha + \rho_0\widehat{w}$ can be decomposed into $L^1(\mathbb{R}^3) + L^2(\mathbb{R}^3)$ and thus, $Q(\alpha + \rho_0\widehat{w})$ is finite and nonnegative by the same reasoning as in (3.10) and (3.13), respectively. Plugging this in, we obtain

$$\begin{aligned} \mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma, \rho_0) &= (2\pi)^{-3} \int_{\mathbb{R}^3} p^2\gamma + \frac{1}{2}\widehat{V}(0)\rho^2 + Q(\alpha + \rho_0\widehat{w}) \\ &- 2\rho_0 Q(\alpha, \widehat{w}) - \rho_0^2 Q(\widehat{w}) + Q(\gamma) + (2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} \widehat{V}(p)(\gamma(p) + \alpha(p))\,\mathrm{d}p \\ &- \Bigg[4\pi a\rho^2 + (2\pi)^{-3} \int_{\mathbb{R}^3} [p^2 + \rho_0\widehat{V}(p)]\gamma(p)\,\mathrm{d}p + (2\pi)^{-3}\frac{\rho_0^2}{2} \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)^2}{2p^2}\,\mathrm{d}p \\ &- (2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} |\widehat{Vu}(p)|\sqrt{\gamma(p)(\gamma(p)+1)}\,\mathrm{d}p + 4\pi(a_0 - a)(\rho^2 - \rho_0^2)\Bigg] \end{aligned} \tag{3.21}$$

We observe that $0 \leqslant Q(\alpha + \rho_0\widehat{w}) = E_2(\gamma, \alpha, \rho_0)$ and that $0 \leqslant Q(\gamma) = E_1(\gamma, \alpha, \rho_0)$ by (3.11). Consider the remaining terms involving α, together with of the first term in the last row of (3.21):

$$(2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} \widehat{V}(p)\alpha(p)\,\mathrm{d}p - 2\rho_0 Q(\alpha, \widehat{w}) + (2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} |\widehat{Vu}(p)|\sqrt{\gamma(p)(\gamma(p)+1)}\,\mathrm{d}p$$

Using (3.20) and $\widehat{Vu} = \widehat{V} - \widehat{Vw}$, we get that this is equal to

$$(2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} \widehat{Vu}(p)\alpha(p) + |\widehat{Vu}(p)|\sqrt{\gamma(p)(\gamma(p)+1)}\,\mathrm{d}p = E_3(\gamma, \alpha, \rho_0)$$

Note that $E_3(\gamma, \alpha, \rho_0) \geqslant 0$ by the definition (3.3) of $\mathcal{D}$. Hence, we arrive at

$$\begin{aligned} \mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma, \rho_0) &= (E_1 + E_2 + E_3)(\gamma, \alpha, \rho_0) + \frac{1}{2}\widehat{V}(0)\rho^2 - \rho_0^2 Q(\widehat{w}) - 4\pi a\rho^2 \\ &- (2\pi)^{-3}\frac{\rho_0^2}{2} \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)^2}{2p^2}\,\mathrm{d}p - 4\pi(a_0 - a)(\rho^2 - \rho_0^2) \end{aligned}$$

Collecting the terms involving ρ in (3.21), and using $4\pi a = \frac{1}{2}\widehat{Vu}(0)$, we get

$$\frac{1}{2}\widehat{V}(0)\rho^2 - 4\pi a\rho^2 - 4\pi(a_0 - a)\rho^2 = 0$$

Using (2.12), we infer

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)^2}{2p^2}\,\mathrm{d}p = \int_{\mathbb{R}^3} \widehat{Vu}(p)\widehat{w}(p)\,\mathrm{d}p &= \int_{\mathbb{R}^3} \widehat{V}(p)\widehat{w}(p)\,\mathrm{d}p - \int_{\mathbb{R}^3} \widehat{Vw}(p)\widehat{w}(p)\,\mathrm{d}p \\ &= (2\pi)^3\widehat{Vw}(0) - 2 \cdot Q(\widehat{w}) \end{aligned}$$

Thus, we arrive at

$$\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma, \rho_0) = (E_1 + E_2 + E_3)(\gamma, \alpha, \rho_0)$$

Since all the error terms are nonnegative, the lemma follows. □

Remark 3.3. We want to explain the choice of $\rho_0\widehat{w}$, which we compare to α in (3.19). Recall from (2.8) that $\widehat{w}$ is the scattering solution in momentum space. Physically, we expect that most of the particles are in the condensate, and that exchange of momentum with the excited particles happens only at a very limited level. Due to the diluteness of the gas, exchange of momentum is mostly given by two-particle scattering and this is what the scattering solution models. The factor of ρ_0 is then reflecting the combinatorical degeneracy for exchanging momentum with the condensate.

3.3 Minimization of the simplified functional

In this subsection, we minimize the simplified functional (3.15) over γ. We first need to extract the integral terms of $\mathcal{F}^{\mathrm{sim}}$. To do this, let $(\gamma,\rho_0)\in\mathcal{D}'$ as in (3.14) and define

$$\begin{aligned}\mathcal{F}^{\mathrm{s}}(\gamma,\rho_0) := (2\pi)^{-3}\int_{\mathbb{R}^3}\Big\{&[p^2+\rho_0\widehat{V}(p)]\gamma(p)-\rho_0|\widehat{Vu}(p)|\sqrt{\gamma(p)(\gamma(p)+1)}\\ &+\frac{\rho_0^2}{2}\frac{\widehat{Vu}(p)^2}{2p^2}\Big\}\mathrm{d}p.\end{aligned}\tag{3.22}$$

Then, using (3.15),

$$\mathcal{F}^{\mathrm{sim}}(\gamma,\rho_0) = 4\pi a\rho^2 + 4\pi(a_0-a)(\rho^2-\rho_0^2)+\mathcal{F}^{\mathrm{s}}(\gamma,\rho_0).\tag{3.23}$$

We start with the minimization of $\mathcal{F}^{\mathrm{s}}$. In Lemma 3.4 below, we enforce the constraint $\rho=\rho_0+\rho_\gamma$ by using a Lagrange multiplier $\delta\geqslant 0$. Note that $\delta=0$ corresponds to unconstrained minimization, i.e., minimization over *all* $\gamma\in L^1((1+p^2)\mathrm{d}p)$ disregarding the constraint (3.4), i.e., $\rho_\gamma=\rho-\rho_0$. We eventually show that this gives a minimizing energy which is too high compared to having $\delta>0$. We justify a posteriori in Subsection 3.6 that δ can be chosen nonnegative. For notational convenience, we define

$$A_\delta(p,\rho_0) := p^2+\delta+\rho_0\widehat{V}(p),\qquad B(p,\rho_0):=\rho_0|\widehat{Vu}(p)|,$$

and

$$\begin{aligned}G_\delta(p,\rho_0) &:= \sqrt{A_\delta(p,\rho_0)^2-B(p,\rho_0)^2}\\ &= \sqrt{(p^2+\delta)^2+2\rho_0(p^2+\delta)\widehat{V}(p)+\rho_0^2[\widehat{V}(p)^2-\widehat{Vu}(p)^2]}\end{aligned}\tag{3.24}$$

Lemma 3.4. *Let Assumption* 1.2 *for* V *be satisfied. There is a* $\widetilde{\rho}_0>0$ *such that, for every* $0\leqslant\rho_0\leqslant\widetilde{\rho}_0$*, the minimizer of*

$$\inf_{\gamma\in L^1((1+p^2)\mathrm{d}p)}\big(\mathcal{F}^{\mathrm{s}}(\gamma,\rho_0)+\delta\rho_\gamma\big)\tag{3.25}$$

is given by

$$\gamma^\delta_{\min}(p) := \frac{1}{2}\bigg(\frac{p^2+\delta+\rho_0\widehat{V}(p)}{G_\delta(p,\rho_0)}-1\bigg),$$

with $G_\delta(p,\rho_0)$ *as in* (3.24)*. The minimum is*

$$\begin{aligned}\mathcal{I}^\delta(\rho_0) &:= \mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\min},\rho_0)+\delta\rho_{\gamma^\delta_{\min}}\\ &= (2\pi)^{-3}\cdot\frac{1}{2}\int_{\mathbb{R}^3}\Big\{G_\delta(p,\rho_0)-p^2-\delta-\rho_0\widehat{V}(p)+\rho_0^2\frac{\widehat{Vu}(p)^2}{2p^2}\Big\}\,\mathrm{d}p\end{aligned}\tag{3.26}$$

Proof. We start by remarking that $G_\delta(p,\rho_0)$ in (3.24) is real provided $\rho_0 \geqslant 0$ is small enough. However, we postpone the argument until the proof of Theorem 3.6 below. Fix $p \in \mathbb{R}^3$ and set $x := \gamma(p)$, so that $x \geqslant 0$, see (3.14). Without loss, assume that $x > 0$. Then, the integrand in $\mathcal{F}^{\mathrm{s}}(\gamma,\rho_0)$ is given by

$$f(x) := A(p,\rho_0)x - B(p,\rho_0)\sqrt{x(x+1)} + \frac{\rho_0^2}{2}\frac{\widehat{Vu}(p)^2}{p^2}.$$

We get that

$$f'(x) = A(p,\rho_0) - \frac{1}{2}B(p,\rho_0)\frac{1+2x}{\sqrt{x(x+1)}} = 0$$

if and only if

$$4A^2 \cdot (x^2+x) = B^2(1+4x+4x^2). \tag{3.27}$$

That is, taking into account the constraint $x \geqslant 0$:

$$x_{\min} = -\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{B^2}{4(A^2-B^2)}} = -\frac{1}{2} + \frac{1}{2}\frac{A}{\sqrt{A^2-B^2}}. \tag{3.28}$$

Considering the second derivative,

$$f''(x) = -\frac{\rho_0|\widehat{Vu}(p)|}{2}\frac{2\cdot\sqrt{x(x+1)} - (1+2x)\cdot\frac{1+2x}{2\sqrt{x(x+1)}}}{x(x+1)} = \frac{|\widehat{Vu}(p)|}{4\sqrt{x(x+1)}^3} \geqslant 0,$$

we get that this is indeed a minimum (except when $\widehat{Vu}(p) = 0$ but then, the obvious minimizer $\gamma(p) = 0$ coincides with our choice). Thus, the minimizing $\gamma^\delta_{\min}$ is given by

$$\gamma^\delta_{\min}(p) = \frac{1}{2}\left(\frac{p^2+\delta+\rho_0\widehat{V}(p)}{G_\delta(p,\rho_0)} - 1\right).$$

Furthermore, from (3.27) and (3.28), we get that

$$\sqrt{\gamma^\delta_{\min}(\gamma^\delta_{\min}+1)} = \frac{B}{2A_\delta}(1+2\gamma^\delta_{\min}) = \frac{B}{2A_\delta}\frac{A_\delta}{\sqrt{A_\delta^2-B^2}} = \frac{B}{2\sqrt{A_\delta^2-B^2}}. \tag{3.29}$$

Hence, the minimal energy is given by

$$\begin{aligned}\mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\min},\rho_0) &= (2\pi)^{-3}\cdot\frac{1}{2}\int_{\mathbb{R}^3}\left\{\frac{A_\delta(p,\rho_0)^2}{G_\delta(p,\rho_0)} - A_\delta(p,\rho_0) - \frac{B(p,\rho_0)^2}{G_\delta(p,\rho_0)} + \rho_0^2\frac{\widehat{Vu}(p)^2}{2p^2}\right\}\mathrm{d}p\\ &= (2\pi)^{-3}\cdot\frac{1}{2}\int_{\mathbb{R}^3}\left\{G_\delta(p,\rho_0) - p^2 - \delta - \rho_0\widehat{V}(p) + \rho_0^2\frac{\widehat{Vu}(p)^2}{2p^2}\right\}\mathrm{d}p.\end{aligned}$$

We prove that $\gamma^\delta_{\min}$ is an allowed variational function for (3.25) in Theorems 3.6 and 3.9 below. $\square$

It will turn out to be necessary to consider the other component of the state $(\gamma^\delta_{\min},\alpha^\delta_{\min})$ as well. Since the minimization problem in (3.25) gives no restriction on the choice of $\alpha^\delta_{\min}$, we may implement right away that we are looking for a quasi-free state (compare to the discussion below (1.8)). We also need $\alpha^\delta_{\mathrm{min}}$ in the proof of the upper bound later. Therefore, let us define

$$\alpha^\delta_{\mathrm{min}}(p) := -\operatorname{sgn}(\widehat{Vu}(p)) \cdot \sqrt{\gamma^\delta_{\mathrm{min}}(p)(\gamma^\delta_{\mathrm{min}}(p)+1)}. \tag{3.30}$$

Note that, by definition of the sign, $\operatorname{sgn}(\widehat{Vu}(p))|\widehat{Vu}(p)| = \widehat{Vu}(p)$ and recall from (3.29) that, therefore,

$$\alpha^\delta_{\mathrm{min}}(p) = -\frac{\rho_0 \widehat{Vu}(p)}{2\sqrt{(p^2+\delta)^2 + 2\rho_0(p^2+\delta)\widehat{V}(p) + \rho_0^2[\widehat{V}(p)^2 - \widehat{Vu}(p)^2]}}.$$

In view of the error term E_3, we need to estimate the integral of $\alpha_{\mathrm{min}} + \rho_0\widehat{w}$. For that purpose, define

$$\mathcal{J}^\delta(\rho_0) := (2\pi)^{-3}\int_{\mathbb{R}^3} |\alpha^\delta_{\mathrm{min}}(p) + \rho_0\widehat{w}(p)|\,\mathrm{d}p.$$

Before we prove that γ_{min} is a valid testfunction for the variational problem (3.25), we rewrite the occuring integrals in a more convenient way.

Corollary 3.5. *Let $\rho_0 \geqslant 0$ and $\phi := (\rho_0\widehat{Vu(0)})^{1/2} \geqslant 0$ be small enough. Let $\delta \geqslant 0$ and set $d := \delta/\phi^2$. Then, we have*

$$\rho_{\gamma^\delta_{\mathrm{min}}} = (2\pi)^{-3}\frac{\phi^3}{2}\int_{\mathbb{R}^3}\left\{\frac{p^2+d+\frac{\widehat{V}(\phi p)}{8\pi a}}{\sqrt{(p^2+d)^2 + 2(p^2+d)\frac{\widehat{V}(\phi p)}{8\pi a} + \frac{\widehat{V}(\phi p)^2}{(8\pi a)^2} - \frac{\widehat{Vu}(\phi p)^2}{(8\pi a)^2}}} - 1\right\}\mathrm{d}p, \tag{3.31}$$

and

$$\mathcal{J}^\delta(\rho_0) = (2\pi)^{-3}\frac{\phi^3}{2}\int_{\mathbb{R}^3}\left|\frac{\widehat{Vu}(\phi p)}{8\pi a}\frac{1}{p^2} - \frac{\frac{\widehat{Vu}(\phi p)}{8\pi a}}{\sqrt{(p^2+d)^2 + 2(p^2+d)\frac{\widehat{V}(\phi p)}{8\pi a} + \frac{\widehat{V}(\phi p)^2}{(8\pi a)^2} - \frac{\widehat{Vu}(\phi p)^2}{(8\pi a)^2}}}\right|\mathrm{d}p, \tag{3.32}$$

and finally

$$\begin{aligned}\mathcal{I}^\delta(\rho_0) = (2\pi)^{-3}\frac{\phi^5}{2}\int_{\mathbb{R}^3}\Bigg\{&\sqrt{(p^2+d)^2 + 2(p^2+d)\frac{\widehat{V}(\phi p)}{8\pi a} + \frac{\widehat{V}(\phi p)^2}{(8\pi a)^2} - \frac{\widehat{Vu}(\phi p)^2}{(8\pi a)^2}} \\ &- p^2 - d - \frac{\widehat{V}(\phi p)}{8\pi a} + \frac{1}{2p^2}\frac{\widehat{Vu}(\phi p)^2}{(8\pi a)^2}\Bigg\}\,\mathrm{d}p.\end{aligned} \tag{3.33}$$

Note that ϕ is reflecting the dilute limit in (1.9) and (1.14).

3.4 Approximation to integrals

We prove that $\gamma^\delta_{\mathrm{min}}$ is an allowed testfunction for the variational problem (3.25). The following integrals will play a prominent role during this analysis. They are defined for $\sigma \in [1,\infty)$:

$$I_1(\sigma) := (2\pi)^{-3}\cdot\frac{1}{2}\int_{\mathbb{R}^3}\left\{\sqrt{p^4+2\sigma p^2+\sigma^2-1} - p^2 - \sigma + \frac{1}{2p^2}\right\}\mathrm{d}p, \tag{3.34}$$

$$I_2(\sigma) := (2\pi)^{-3}\cdot\frac{1}{2}\int_{\mathbb{R}^3}\left\{\frac{p^2+\sigma}{\sqrt{p^4+2\sigma p^2+\sigma^2-1}} - 1\right\}\mathrm{d}p, \tag{3.35}$$

$$I_3(\sigma) := (2\pi)^{-3}\cdot\frac{1}{2}\int_{\mathbb{R}^3}\left\{\frac{1}{p^2} - \frac{1}{\sqrt{p^4+2\sigma p^2+\sigma^2-1}}\right\}\mathrm{d}p. \tag{3.36}$$

Note that $I_1 = I$ as in (1.15) but from now on we carry the enumeration for notational convenience and clarity.

Theorem 3.6. *Let $\rho_0, \delta \geqslant 0$ and define $\phi := (\rho_0 \widehat{Vu}(0))^{1/2}$. Assume that V satisfies Assumption* 1.2 *and that $1 < \nu < 3/2$. Then, there is a $\phi_0 > 0$ and $h \in L^1(\mathbb{R}^3)$ such that we have $|\gamma^\delta_{\min}| \leqslant |h|$ for all $0 \leqslant \phi \leqslant \phi_0$ and all $d \geqslant 0$, where $\delta = d\phi^2$. In particular, $\rho_{\gamma^\delta_{\min}}$ is continuous in $\phi \in [0, \phi_0]$ and*

$$\rho_{\gamma^\delta_{\min}} = \phi^3 I_2(\nu + d) + \mathrm{o}(\phi^3) \qquad \text{as } \phi \to 0.$$

The error is uniform in d. Moreover, I_2 is continuous.

Theorem 3.7. *Let $\rho_0, \delta \geqslant 0$ and define $\phi := (\rho_0 \widehat{Vu}(0))^{1/2}$. Assume that V satisfies Assumption* 1.2 *and that $1 < \nu < 3/2$. Let ϕ_0 be as in Theorem* 3.6 *and $d = \delta/\phi^2$. Then, there is $h_d \in L^1(\mathbb{R}^3)$ such that $|\alpha^\delta_{\min} + \rho_0 \widehat{w}| \leqslant |h_d|$ for all $0 \leqslant \phi \leqslant \phi_0$. In particular, $\mathcal{J}$ is continuous in $\phi \in [0, \phi_0]$ and*

$$\mathcal{J}^\delta = \phi^3 I_3(\nu + d) + \mathrm{o}(\phi^3) \qquad \text{as } \phi \to 0.$$

If $d \in [0, d_0]$ for some $d_0 > 0$, then the error is uniform in d. Moreover, I_3 is continuous.

Remark 3.8. Recall that, a priori, $\alpha + \rho_0 \widehat{w}$ could only be decomposed according to $L^1(\mathbb{R}^3) + L^2(\mathbb{R}^3)$, compare (3.19). Applying Theorem 3.7, we realize that, for the minimizer $\alpha^\delta_{\min}$, the situation is better, namely $\alpha^\delta_{\min} + \rho_0 \widehat{w} \in L^1(\mathbb{R}^3)$. The "bad part", where γ is small (see (3.5)), is not present in $\alpha^\delta_{\min}$.

Theorem 3.9. *Let $\rho_0, \delta \geqslant 0$ and define $\phi := (\rho_0 \widehat{Vu}(0))^{1/2}$. Assume that V satisfies Assumption* 1.2 *and that $1 < \nu < 3/2$. Let ϕ_0 be as in Theorem* 3.6 *and $d = \delta/\phi^2$. Then there is $h_d \in L^1(\mathbb{R}^3)$ such that $|p^2 \gamma^\delta_{\min}| \leqslant |h_d|$ for all $0 \leqslant \phi \leqslant \phi_0$. In particular, $\mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\min}, \cdot)$ is continuous in $\phi \in [0, \phi_0]$ and*

$$\mathcal{I}^\delta = \phi^5 I_1(\nu + d) + \mathrm{o}(\phi^5) \qquad \text{as } \phi \to 0.$$

If $d \in [0, d_0]$ for some $d_0 > 0$, then the error is uniform in d. Moreover, I_1 is continuous.

The method of proof of Theorems 3.6, 3.7, and 3.9 is inspired by the proofs of Lemmas 24 and 27 in [3].

Proof of Theorem 3.6. Recall that $|\widehat{Vu}(p)| \leqslant \widehat{Vu}(0) = 8\pi a$ and $|\widehat{V}(p)| \leqslant \widehat{V}(0) = 8\pi a_0$, see (2.9). Also, $\nu = \frac{a_0}{a} > 1$ by the assumption (1.13). We split the integral in (3.31) into two regions, namely $p^2 \leqslant 3$ and $p^2 \geqslant 3$ and start with $p^2 \leqslant 3$. First, let us prove that the term under the square root is nonnegative, compare (3.24). Denote $x := p^2 + d$ and note that the term under the square root is equal to

$$\left(x + \frac{\widehat{V}(\phi p)}{8\pi a}\right)^2 - \left(\frac{\widehat{Vu}(\phi p)}{8\pi a}\right)^2 = \left(x + \frac{\widehat{V}(\phi p)}{8\pi a} + \frac{\widehat{Vu}(p)}{8\pi a}\right)\left(x + \frac{\widehat{V}(\phi p)}{8\pi a} - \frac{\widehat{Vu}(p)}{8\pi a}\right). \quad (3.37)$$

Recall that, by Assumption 1.2 (4), $\widehat{V}$ is differentiable at $p = 0$. Hence

$$C_1 := \sup_{0 \leqslant |p| \leqslant \sqrt{3}} \frac{|\widehat{V}(p) - \widehat{V}(0)|}{|p|} < \infty. \quad (3.38)$$

Choose $\phi_0 := 8\pi a \cdot \frac{\nu-1}{\sqrt{3}\cdot C_1} > 0$. Then, for every $0 \leqslant \phi \leqslant \phi_0$ and each $p \in \mathbb{R}^3$ with $0 \leqslant |p| \leqslant \sqrt{3}$, we can estimate

$$\begin{aligned} x + \frac{\widehat{V}(\phi p)}{8\pi a} \pm \frac{\widehat{Vu}(\phi p)}{8\pi a} &\geqslant x + \frac{\widehat{V}(0)}{8\pi a} - \frac{\widehat{Vu}(0)}{8\pi a} - \left| \frac{\widehat{V}(\phi p) - \widehat{V}(0)}{8\pi a} \right| \\ &\geqslant x + \nu - 1 - \frac{C_1}{8\pi a}|p| \cdot \phi \\ &\geqslant x + \nu - 1 - \frac{\sqrt{3}\cdot C_1}{8\pi a} \cdot 8\pi a \cdot \frac{\nu - 1}{\sqrt{3}\cdot C_1} = p^2 + d. \end{aligned} \tag{3.39}$$

Note that the integrand of (3.31) is nonnegative. Hence, for these p, a dominating function is obtained by choosing ν/p^2. This function is independent of d and integrable at $p = 0$ in 3 dimensions . We turn to the region $|p| \geqslant \sqrt{3}$. To prove integrability here, we consider the integrand

$$f(t,s) := \frac{x+t}{\sqrt{(x+t)^2 - s^2}} - 1$$

on the rectangle $(t,s) \in [-\nu,\nu] \times [-1,1]$. Here $t := \frac{\widehat{V}(p)}{8\pi a}$, $s := \frac{\widehat{Vu}(p)}{8\pi a}$. Note that we assume that $x = p^2 + d \geqslant 3$ so that

$$(x+t)^2 - s^2 = x^2 + 2tx + t^2 - s^2 \geqslant 9 - 6\cdot\nu - 1 \geqslant 0. \tag{3.40}$$

Thus, the square root is always well-defined, since $\nu \leqslant 3/2$ by the assumption (1.13). Also, $f(t,s) \geqslant f(t,0) = 0$ and $f(t,s) \leqslant f(t,1)$. Define $g(t) := f(t,1) = \frac{x+t}{\sqrt{(x+t)^2-1}} - 1$ and maximize over $t \in [-\nu,\nu]$. We have

$$g'(t) = \frac{\sqrt{(x+t)^2-1} - (x+t)\frac{(x+t)}{\sqrt{(x+t)^2-1}}}{(x+t)^2 - 1} = -\frac{1}{\sqrt{(x+t)^2-1}} < 0.$$

Hence, since $g > 0$, the maximal modulus is located at the left boundary $t = -\nu$. In the following, let us consider $g(\pm\nu)$ simultaneously, keeping in mind that we also want to prove well-definedness of $I_2(\sigma)$ in (3.35) for every $\sigma \geqslant 1$. Hence, we need to deal with

$$0 < g(\pm\nu) = \frac{x \pm \nu}{\sqrt{x^2 \pm 2\nu x + \nu^2 - 1}} - 1 \leqslant \frac{x \pm \nu}{\sqrt{x^2 \pm 2\nu x}} - 1$$

since $\nu^2 - 1 > 0$. A simple argument shows that the derivative with respect to d of the right hand side is strictly negative since $\nu \neq 0$. Hence, it is further maximized by choosing $d = 0$. Now, the functions $h_\pm \colon [\sqrt{3/\nu}, \infty) \longrightarrow \mathbb{R}$, given by

$$h_\pm(u) := \frac{u^4 \pm u^2}{\sqrt{u^4 \pm 2u^2}} - u^2,$$

are well-defined since for h_-, we have $\nu < 3/2$, hence $u^4 - 2u^2 \geqslant u^2(\frac{3}{\nu} - 2)$ and h_+ is well-defined without any restriction. If we show that h_- is integrable, then, by the substitution $p = \sqrt{\nu}\cdot q \in \mathbb{R}^3$, we get

$$\begin{aligned} \int_{|p|\geqslant\sqrt{3}} \frac{p^2 - \nu}{\sqrt{p^4 - 2\nu p^2}} - 1 \,\mathrm{d}p &= \nu^{\frac{3}{2}} \int_{|q|\geqslant\sqrt{3/\nu}} \frac{\nu q^2 - \nu}{\sqrt{\nu^2 q^4 - 2\nu^2 q^2}} - 1 \,\mathrm{d}q \\ &= 4\pi\nu^{3/2} \int_{\sqrt{3/\nu}}^\infty \frac{u^4 - u^2}{\sqrt{u^4 - 2u^2}} - u^2 \,\mathrm{d}u = 4\pi\nu^{3/2} \int_{\sqrt{3/\nu}}^\infty h(u)\,\mathrm{d}u. \end{aligned} \tag{3.41}$$

Hence, when h_+ is shown to be integrable, well-definedness and continuity of I_2 is proved. Thus, we are concerned with proving that $h_\pm$ are integrable. To see this, note that a primitive is given by $H_\pm \colon [\sqrt{3/\nu}, \infty) \longrightarrow \mathbb{R}$,

$$H_\pm(u) := \frac{u^4 \pm u^2 - 2}{3\sqrt{u^2 \pm 2}} - \frac{u^3}{3},$$

because for each $u \in [\sqrt{3/\nu}, \infty)$, we have:

$$\begin{aligned} H'_\pm(u) &= \frac{3(4u^3 \pm 2u)\sqrt{u^2 \pm 2} - 3(u^4 \pm u^2 - 2) \cdot \frac{2u}{2\sqrt{u^2 \pm 2}}}{9(u^2 \pm 2)} - u^2 \\ &= \frac{1}{3\sqrt{u^2 \pm 2}^3}\Big[(4u^3 \pm 2u)(u^2 \pm 2) - (u^4 \pm u^2 - 2)u\Big] - u^2 \\ &= \frac{1}{\sqrt{u^2 \pm 2}^3}(u^5 \pm 3u^2 - 2u) - u^2 = \frac{u}{\sqrt{u^2 \pm 2}^3}(u^2 \pm 2)(u^2 - 1) - u^2 = h_\pm(u). \end{aligned}$$

We are left with proving that $H_\pm(u) \xrightarrow{u \to \infty} 0$. Write

$$H_\pm(u) = \frac{u^4 \pm u^2 - 2 - u^3\sqrt{u^2 \pm 2}}{3\sqrt{u^2 \pm 2}}$$

and apply l'Hôpital's rule multiple times. In the limit $u \to \infty$, we may consider equivalently

$$\begin{aligned} \widetilde{H}_\pm(u) &= \frac{4u^3 \pm 2u - 3u^2\sqrt{u^2 \pm 2} - u^3 \cdot \frac{u}{\sqrt{u^2 \pm 2}}}{\frac{3u}{\sqrt{u^2 \pm 2}}} = \frac{1}{3}\Big[(4u^2 \pm 2)\sqrt{u^2 \pm 2} - 4u^3 + 6u\Big] \\ &= \mp\frac{2}{3}(u - \sqrt{u^2 \pm 2}) + \frac{4}{3}(u^2\sqrt{u^2 \pm 2} - u^3 \mp u) =: \mp\frac{2}{3} \cdot \widetilde{H}_1(u) + \frac{4}{3} \cdot \widetilde{H}_2(u), \end{aligned}$$

where we dropped the $(\pm)$-dependence in the definition of $\widetilde{H}_1$ and $\widetilde{H}_2$. We shall prove in the following that $\widetilde{H}_1(u)$ and $\widetilde{H}_2(u)$ vanish at infinity independently. We start with $\widetilde{H}_1$ and notice that, for large $u > 0$,

$$\widetilde{H}_1(u) = u - \sqrt{u^2 \pm 2} = u(1 - \sqrt{1 \pm 2/u^2}) = \frac{1 - \sqrt{1 \pm 2/u^2}}{1/u}.$$

By l'Hôpital's rule, we get the equivalent expression

$$\frac{\mp\frac{1}{2\sqrt{1 \pm 2/u^2}} \cdot \frac{4}{u^3}}{-1/u^2} = \frac{\pm 2}{\sqrt{u^2 - 2}} \xrightarrow{u \to \infty} 0.$$

Hence, the claim holds for $\widetilde{H}_1$. To continue with $\widetilde{H}_2$, we use the same strategy to get

$$\widetilde{H}_2(u) = u^3\left(\sqrt{1 \pm \frac{2}{u^2}} - 1 \mp \frac{1}{u^2}\right) = \frac{\sqrt{1 \pm 2/u^2} - 1 \mp 1/u^2}{1/u^3}.$$

In the limit $u \to \infty$, by l'Hôpital's rule, this is equivalent to

$$\frac{\frac{\mp 4/u^3}{2\sqrt{1 \pm 2/u^2}} \cdot \pm 2/u^3}{-3/u^4} = \pm\frac{2}{3}\left(\frac{u}{\sqrt{1 \pm 2/u^2}} - u\right) =: \pm\frac{2}{3} \cdot \widetilde{H}_3(u).$$

Applying this trick a last time to $\widetilde{H}_3(u)$, we get the equivalent expression

$$\frac{\frac{\pm 2}{u^3\sqrt{1\pm 2/u^2}^3}}{-1/u^2} = \mp 2 \cdot \frac{1}{\sqrt{u^2 \pm 2}} \xrightarrow{u\to\infty} 0$$

in the limit $u \to \infty$. The rest is an application of Lebesgue's Dominated Convergence Theorem. Use (3.37) to get that the pointwise limit as $\phi \to 0$ in the integrand of (3.31) is $I_2(\nu + d)$ from (3.35). ☐

Proof of Theorem 3.7. We proceed analogously to the proof of Theorem 3.6 and split the integration region in (3.32) into $p^2 \leqslant 3$ and $p^2 \geqslant 3$. Recall that with the choice of $\phi_0 > 0$ in the proof of Theorem 3.6, the square root is well-defined for all $0 \leqslant \phi \leqslant \phi_0$, see (3.39). Note again that $\frac{1}{p^2}$ is integrable at $p = 0$ in 3 dimensions. Hence, for $p^2 \leqslant 3$, we obtain a dominating function for the integrand by maximizing each term separately. For $p^2 \geqslant 3$ the square root is well-defined by (3.40). Consider the integrand

$$\left|\frac{s}{p^2} - \frac{s}{\sqrt{(x+t)^2 - s^2}}\right| \leqslant \left|\frac{1}{p^2} - \frac{1}{\sqrt{(x+t)^2 - s^2}}\right| =: |f(t,s)|$$

in the rectangle $(t, s) \in [-\nu, \nu] \times [-1, 1]$ with, again, $x = p^2 + d$, $t = \frac{\widehat{V}(\phi p)}{8\pi a}$, and $s = \frac{\widehat{Vu}(\phi p)}{8\pi a}$. We have

$$\frac{\partial f}{\partial t}(t,s) = \frac{x+t}{\sqrt{(x+t)^2 - s^2}} \qquad \frac{\partial f}{\partial s}(t,s) = -\frac{s}{\sqrt{(x+t)^2 - s^2}}.$$

Since $\nu < 3$, we have that $x + t \neq 0$ for all $t \in [-\nu, \nu]$ and hence, f has no critical point in the rectangle. Thus, the maximal modulus is attained at the boundary and, due to the symmetry of f in s, we need to consider the functions

$$g_1(t) := \frac{1}{p^2} - \frac{1}{\sqrt{(x+t)^2 - 1}} \qquad g_\pm(s) := \frac{1}{p^2} - \frac{1}{\sqrt{(x \pm \nu)^2 - s^2}}.$$

As in the previous proof, one shows that both functions attain their maximal modulus at the boundary and hence, we are left with the two candidates

$$\frac{1}{p^2} - \frac{1}{\sqrt{(x \pm \nu)^2 - 1}}$$

as maximizers. Now, with $\eta := d \pm \nu$, define $h_\pm \colon [\sqrt{3/\nu}, \infty) \longrightarrow \mathbb{R}$ by

$$h_\pm(u) := 1 - \frac{u^2}{\sqrt{u^4 + 2\eta u^2 + \eta^2 - 1}},$$

reflecting the choice of polar coordinates similarly to (3.41). For each $0 < \varepsilon < 1$, we show that $u^{1+\varepsilon} h_\pm(u) \to 0$ as $u \to \infty$. In preparation, define

$$r_\pm(u) := \sqrt{1 + \frac{2\eta}{u^2} + \frac{\eta^2 - 1}{u^4}} \tag{3.42}$$

for $u > 0$ large enough. By applying l'Hôpital's rule, we get $u^{1+\varepsilon} h_\pm(u) = u^{1+\varepsilon}[1 - r_\pm(u)^{-1}]$, so that it suffices to consider

$$\frac{2}{r_\pm(u)^3} \frac{-\frac{\eta}{u^3} - \frac{\eta^2-1}{u^5}}{-\frac{1+\varepsilon}{u^{2+\varepsilon}}} = \frac{1}{1+\varepsilon} \frac{2}{r_\pm(u)^3} \left(\frac{\eta}{u^{1-\varepsilon}} + \frac{\eta^2 - 1}{u^{3-\varepsilon}}\right) \xrightarrow{u\to\infty} 0$$

The rest is an application of dominated convergence. Use (3.37) to get that the pointwise limit as $\phi \to 0$ in the integrand of (3.32) is $I_3(\nu + d)$ from (3.36). If $d \in [0, d_0]$ for some $d_0 > 0$, we may maximize the dominating function further by replacing d with d_0. In this way, we get uniform convergence in d as $\phi \to 0$. $\square$

Proof of Theorem 3.9. We intend to prove that $p^2\gamma^\delta_{\min}$ is integrable. From Theorem 3.6, we know that $\gamma^\delta_{\min} \in L^1(\mathbb{R}^3)$. By the same reasoning as below (3.15), we get that

$$\int_{\mathbb{R}^3} |\widehat{Vu}(p)| \sqrt{\gamma^\delta_{\min}(p)(\gamma^\delta_{\min}(p)+1)}\,\mathrm{d}p < \infty.$$

Using (2.7), we infer that all terms in $\mathcal{F}^{\mathrm{s}}$ in (3.22) are finite except the term with $p^2\gamma^\delta_{\min}$. Hence, recalling (3.26), it is enough to prove that $\mathcal{I}^\delta = \mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\min}, \cdot)$ has the required properties of the theorem. We use the by now familiar split into $p^2 \leqslant 3$ and $p^2 \geqslant 3$. Again, the square root is well-defined in both regimes because of (3.39) and (3.40). The integrand is given by

$$f(t,s) = \sqrt{(x+t)^2 - s^2} - x - t + \frac{s^2}{2p^2}, \qquad (t,s) \in [-\nu,\nu] \times [-1,1],$$

where $x = p^2 + d$, $t = \frac{\widehat{V}(\phi p)}{8\pi a}$, and $s = \frac{\widehat{Vu}(\phi p)}{8\pi a}$. Note that, for $p^2 \leqslant 3$, a dominating function is obtained by maximizing the absolute value of each term in t and s separately. We turn to the region $p^2 \geqslant 3$ and calculate

$$\frac{\partial f}{\partial t}(t,s) = \frac{x+t}{\sqrt{(x+t)^2 - s^2}} - 1, \qquad \frac{\partial f}{\partial s}(t,s) = \frac{-s}{\sqrt{(x+t)^2 - s^2}} + \frac{s}{p^2}.$$

We see that $\frac{\partial f}{\partial t}$ vanishes if and only if $s = 0$. Here, $\frac{\partial f}{\partial s}(t,0) = 0$ and also $f(t,0) = 0$. Hence, the maximum of $|f(t,s)|$ is located at the boundary and it suffices to consider the functions

$$\begin{aligned} g_1(t) &:= \sqrt{(x+t)^2 - 1} - x - t + \frac{1}{2x}, && t \in [-\nu,\nu], \\ g_\pm(s) &:= \sqrt{(x\pm\nu)^2 - s^2} - x \mp \nu + \frac{s^2}{2x}, && s \in [-1,1]. \end{aligned}$$

An elementary analysis using the assumption that $\nu < 3/2$ shows that all these functions attain their maximal modulus at the boundary. Hence, we are left with the two candidates

$$\sqrt{(x\pm\nu)^2 - 1} - x \mp \nu + \frac{1}{2x}$$

as maximizers. Now, define $h_\pm \colon [\sqrt{3/\nu}, \infty) \longrightarrow \mathbb{R}$ by

$$h_\pm(u) := u^2\sqrt{(u^2+\eta)^2 - 1} - u^4 - \eta u^2 + \frac{1}{2}$$

reflecting the choice of polar coordinates and using $\eta = d \pm \nu$. Again, we show that, for any $0 < \varepsilon < 1$, we have $u^{1+\varepsilon}h_\pm(u) \to 0$ as $u \to \infty$, proving that $h_\pm$ is integrable. The rest is an application of dominated convergence. Recall $r_\pm(u)$ from (3.42), which tends to 1 as $u \to \infty$. As before, we are going to use l'Hôpital's rule 3 times. The object of interest is

$$u^{1+\varepsilon}h_\pm(u) = u^{5+\varepsilon}\Big[r_\pm(u) - 1 - \frac{\eta}{u^2} + \frac{1}{2u^4}\Big] = \frac{r_\pm(u) - 1 - \frac{\eta}{u^2} + \frac{1}{2u^4}}{\frac{1}{u^{5+\varepsilon}}}.$$

Written in this way, we see that l'Hôpital's rule is applicable and that we can equivalently consider

$$\frac{\frac{-\frac{4\eta}{u^3}-\frac{4(\eta^2-1)}{u^5}}{2r_\pm(u)}+\frac{2\eta}{u^3}-\frac{2}{u^5}}{-\frac{5+\varepsilon}{u^{6+\varepsilon}}}=\frac{u^{3+\varepsilon}}{5+\varepsilon}\left[\frac{2\eta+\frac{2(\eta^2-1)}{u^2}}{r_\pm(u)}-2\eta+\frac{2}{u^2}\right]$$

in the limit $u\to\infty$. We see that we may apply it once more to get (omitting $\frac{1}{5+\varepsilon}$):

$$\frac{-\frac{4(\eta^2-1)}{u^3 r_\pm(u)}+4\frac{(\eta+(\eta^2-1)/u^2)^2}{u^3 r_\pm(u)^3}-\frac{4}{u^3}}{-\frac{3+\varepsilon}{u^{4+\varepsilon}}}=\frac{u^{1+\varepsilon}}{3+\varepsilon}\left[\frac{4(\eta^2-1)}{r_\pm(u)}-\frac{4}{r_\pm(u)^3}\left(\eta+\frac{\eta^2-1}{u^2}\right)^2+4\right].$$

Note that the term in the square brackets tends to 0 as $u\to\infty$. Again, omitting $\frac{1}{3+\varepsilon}$ and applying l'Hôpital's rule a third time, we may consider:

$$\begin{aligned}&\frac{-\frac{2(\eta^2-1)}{r_\pm(u)^3}\left(-\frac{4\eta}{u^3}-\frac{4(\eta^2-1)}{u^5}\right)+\frac{16}{u^3 r_\pm(u)^3}\left(\pm\eta+\frac{\eta^2-1}{u^2}\right)(\eta^2-1)-\frac{24}{u^3 r_\pm(u)^5}\left(\eta+\frac{\eta^2-1}{u^2}\right)^3}{-\frac{1+\varepsilon}{u^{2+\varepsilon}}}\\
&=\frac{1}{1+\varepsilon}\left[\frac{2(\eta^2-1)}{r_\pm(u)^3}\left(-\frac{4\eta}{u^{1-\varepsilon}}-\frac{4(\eta^2-1)}{u^{3-\varepsilon}}\right)-\frac{16}{r_\pm(u)^3}\left(\eta+\frac{\eta^2-1}{u^2}\right)\frac{\eta^2-1}{u^{1-\varepsilon}}\right.\\
&\qquad\left.-\frac{24}{u^{1-\varepsilon}r_\pm(u)^5}\left(\eta+\frac{\eta^2-1}{u^2}\right)^3\right]\end{aligned}$$

and the last expression goes to 0 as $u\to\infty$. Use (3.37) to get that the pointwise limit as $\phi\to 0$ in the integrand of (3.33) is $I_1(\nu+d)$ from (3.34). If $d\in[0,d_0]$ for some $d_0>0$, we may maximize the dominating function further by replacing d with d_0. In this way, we get uniform convergence in d as $\phi\to 0$. □

Corollary 3.10. *We have* $I_2(1)=\frac{\sqrt{2}}{12\pi^2}$.

Proof. In the proof of Theorem 3.6, the primitive of the integrand in (3.35),

$$H(u)=\frac{u^4+u^2-2}{3\sqrt{u^2+2}}-u,$$

is shown to vanish at infinity. Hence, $I_2(1)=-\frac{1}{2(2\pi)^3}\cdot 4\pi\cdot H(0)$. □

Corollary 3.11. *We have* $I_1(1)=\frac{2\sqrt{2}}{15\pi^2}$.

Proof. In this special case $\sigma=1$, a primitive for the integrand in (3.34) is given by $H\colon[0,\infty)\longrightarrow\mathbb{R}$,

$$H(u):=\frac{u}{2}-\frac{u^3}{3}-\frac{u^5}{5}+\sqrt{u^2+2}\left(\frac{u^4}{5}+\frac{2u^2}{15}-\frac{8}{15}\right),$$

since

$$\begin{aligned}H'(u)&=\frac{1}{2}-u^2-u^4+\frac{u}{\sqrt{u^2+2}}\left(\frac{u^4}{5}+\frac{2u^2}{15}-\frac{8}{15}\right)+\sqrt{u^2+2}\left(\frac{4u^3}{5}+\frac{4u}{15}\right)\\&=\frac{1}{2}-u^2-u^4+\frac{1}{\sqrt{u^2+2}}\cdot u^3(u^2+2)=\frac{1}{2}-u^2-u^4+u^2\sqrt{u^4+2u^2}.\end{aligned}$$

The proof of Theorem 3.9 shows that $H(u)\to 0$ as $u\to\infty$. Hence,

$$\int_0^\infty\left\{u^2\sqrt{u^4+2u^2}-u^4-u^2+\frac{1}{2}\right\}\mathrm{d}u=-H(0)=\frac{8}{15}\cdot\sqrt{2}.$$ □

Corollary 3.12. *The integral I_1 is continuously differentiable on $[1,\infty)$ and $I_1'(\sigma) = I_2(\sigma)$ holds for each $\sigma \in [1,\infty)$. Moreover, $I_2(\sigma) > 0$ for all $\sigma \in [1,\infty)$. In particular, I_1 is strictly monotonically increasing.*

Proof. Let $\sigma \in [1,\infty)$ and $h \neq 0$ small enough (if $\sigma = 1$, we require $h > 0$). Consider the difference quotient

$$\frac{I_1(\sigma+h) - I_1(\sigma)}{h} = \\ = \frac{1}{2(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{h} \Big\{ \sqrt{p^4 + 2(\sigma+h)p^2 - (\sigma+h)^2 - 1} - \sqrt{p^4 + 2\sigma p^2 + \sigma^2 - 1} + h \Big\} \, \mathrm{d}p.$$

By the mean value theorem, the integrand is equal to the integrand in $I_2(\eta)$ for some $\eta \in [\sigma - h, \sigma + h]$ (or, $[1, 1+h]$ in case $\sigma = 1$). Hence, dominated convergence applies and we get that $I_1'(\sigma) = I_2(\sigma)$ for every $\sigma \in [1,\infty)$. That $I_2(\sigma) \geqslant 0$ is obtained by pointwise estimating the integrand. If it was zero, the integrand would need to be zero, a contradiction. ☐

3.5 Estimates for the minimizer

In the following, we want to prepare the proof of our main theorem, Theorem 1.3. The preceding section was devoted to find lower bounds on the functional $\mathcal{F}^{\mathrm{can}}$. Now, we are concerned with the upper bound for which we need to take a suitable trial state $(\gamma, \alpha, \rho_0) \in \mathcal{D}$ and compute $\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0)$. We present our choice of trial state right away. For γ, we take the minimizing $\gamma^\delta_{\mathrm{min}}$ from Lemma 3.4. Then, Theorems 3.6 and 3.9 tell us that this is an allowed trial state, i.e., $\gamma^\delta_{\mathrm{min}} \geqslant 0$ and $\gamma^\delta_{\mathrm{min}} \in L^1((1+p^2)\mathrm{d}p)$ provided $\rho_0 \geqslant 0$ is small enough. This choice is reasonable, since $\gamma^\delta_{\mathrm{min}}$ minimizes $\mathcal{F}^{\mathrm{s}}$. Therefore, it should serve as a good upper bound as well. For α, we take $\alpha^\delta_{\mathrm{min}}$ as defined in (3.30). Let us try to motivate this choice a little bit. The Bogolubov Hamiltonian associated to $H_{N,L}$ from (1.1), which is quadratic, has a quasi-free ground state[8]. As mentioned in the introduction, quasi-free states satisfy $\alpha^2 = \gamma(\gamma+1)$, which is a strong motivation for the choice of α. Moreover, we have discussed below (1.7) that α has the interpretation to describe long range interaction between the particles which is believed to exist in a condensed gas. This is why we choose $\alpha^\delta_{\mathrm{min}}$ to have the maximal possible modulus allowed in $\mathcal{D}$. The factor in front is designed to drive the error term E_3 in (3.18) to 0.

Lemma 3.13. *Assume that V satisfies Assumption 1.2, that $1 < \nu < 3/2$, and that $\delta \geqslant 0$. As $\rho a \to 0$, we have that*

$$(E_1 + E_2 + E_3)(\gamma^\delta_{\mathrm{min}}, \alpha^\delta_{\mathrm{min}}, \rho_0) = \mathrm{o}(\rho a)^{5/2},$$

where E_1, E_2, and E_3 are from (3.16), (3.17), and (3.18), respectively.

Proof. Notice that our choice of trial function implies that $E_3(\gamma^\delta_{\mathrm{min}}, \alpha^\delta_{\mathrm{min}}, \rho_0) = 0$ since the integrand is identically 0, see (3.18). Concerning E_1 from (3.16), we have, using (3.9) and Theorem 3.6, that

$$E_1(\gamma^\delta_{\mathrm{min}}, \alpha^\delta_{\mathrm{min}}, \rho_0) \leqslant \widehat{V}(0)\rho^2_{\gamma^\delta_{\mathrm{min}}} \leqslant \widehat{V}(0)(8\pi a\rho_0)^3 + \mathrm{o}(a\rho_0)^3 \leqslant \mathrm{o}(\rho a)^{5/2}.$$

Using Theorem 3.7, the same trick works for E_2 in (3.17):

$$E_2(\gamma^\delta_{\mathrm{min}}, \alpha^\delta_{\mathrm{min}}, \rho_0) \leqslant \frac{1}{2}\widehat{V}(0)\mathcal{J}(\rho_0)^2 \leqslant C\rho_0^3 + \mathrm{o}(a\rho_0)^3 \leqslant \mathrm{o}(\rho a)^{5/2}.$$ ☐

[8] The reader is referred to Chapters 11 and 13.1 of [5] for a detailed discussion of quadratic Hamiltonians in general and the Bogolubov Hamiltonian in particular.

Note that the error is not yet uniform in $\delta \geqslant 0$ because we do not yet know that δ lives in a bounded domain. We need another technical lemma which will help us to prove that the error is uniform in δ. It is a version of Lemma 33 in [3].

Lemma 3.14 [3, Lemma 33]**.** *Let $\rho_0 \geqslant 0$, $\delta \geqslant 0$ and $d = \delta/\phi^2$. For $d \gg 1$, we have*

$$\mathcal{I}(\rho_0) - d\phi^2 \rho_{\gamma^\delta_{\min}} \geqslant C(a) \min\{d^{1/2}(\rho_0 a)^{5/2}, (\rho_0 a)^2\}$$

Furthermore, $\rho_{\gamma^\delta_{\min}} \to 0$ as $d \to \infty$.

Proof. Consider $\mathcal{I}^\delta(\rho_0)$ from (3.33) and write $A(p) := \frac{\widehat{V}(\phi p)}{8\pi a}$ as well as $B(p) = \frac{\widehat{Vu}(\phi p)}{8\pi a}$. For $d \gg 1$, by using l'Hôpital's rule, expand according to

$$(p^2+d)\sqrt{1 + \frac{2A}{p^2+d} + \frac{A^2 - B^2}{(p^2+d)^2}} = p^2 + d + A - \frac{B^2}{2(p^2+d)} + \mathrm{o}(p^2+d)^{-1}.$$

We infer that the asymptotic behavior of $\mathcal{I}^\delta(\rho_0)$ is

$$(2\pi)^{-3}\phi^5 \frac{1}{4}\int_{\mathbb{R}^3} \frac{B(p)^2}{p^2} - \frac{B(p)^2}{2(p^2+d)}\,\mathrm{d}p = (2\pi)^{-3} d\phi^5 \frac{1}{4}\int_{\mathbb{R}^3} \frac{B(p)^2}{p^2(p^2+d)}\,\mathrm{d}p. \tag{3.43}$$

In the same spirit, we can expand the integrand in $\rho_{\gamma^\delta_{\min}}$ from (3.31) to get

$$\frac{p^2+d+A}{\sqrt{(p^2+d)^2 + 2(p^2+d)A + B}} - 1 = \frac{B^2}{2(p^2+d)^2} + \mathrm{o}(p^2+d)^{-2},$$

so that the asymptotic behavior of $-d\phi^2\rho_{\gamma^\delta_{\min}}$ is

$$-(2\pi)^{-3} d\phi^5 \frac{1}{4}\int_{\mathbb{R}^3} \frac{B^2}{(p^2+d)^2}\,\mathrm{d}p. \tag{3.44}$$

Hence, the sum of the two contributions (3.43) and (3.44) is

$$(2\pi)^{-3} d^2\phi^5 \frac{1}{4}\int_{\mathbb{R}^3} \frac{B(p)^2}{p^2(p^2+d)^2}\,\mathrm{d}p = (2\pi)^{-3} d^{1/2}\phi^5 \frac{1}{4}\int_{\mathbb{R}^3} \frac{\widehat{Vu}(d^{1/2}\phi p)^2 (8\pi a)^{-2}}{p^2(p^2+1)^2}\,\mathrm{d}p. \tag{3.45}$$

Recall that, since $\widehat{Vu}$ is differentiable, $C_1 < \infty$ in (3.38). Hence, in the region where $|p| \leqslant \min\{\frac{4\pi a}{C_1}, \sqrt{3}\} =: C_0(a)$, we have $\widehat{Vu}(p) \geqslant 4\pi a$. If $d^{1/2}\phi \leqslant 1$ then the right hand side of (3.45) is bounded from below by

$$(2\pi)^{-3} d^{1/2}\phi^5 \frac{1}{4}\int_{|p|\leqslant C_0} \frac{\widehat{Vu}(d^{1/2}\phi p)^2 (8\pi a)^{-2}}{p^2(p^2+1)^2}\,\mathrm{d}p \geqslant C(a) d^{1/2}\phi^5.$$

If $d^{1/2}\phi \geqslant 1$, the left hand side of (3.45) is bounded from below as

$$(2\pi)^{-3}\phi^4 \frac{1}{4}\int_{\mathbb{R}^3} \frac{\widehat{Vu}(p)(8\pi a)^{-2}}{p^2(\frac{p^2}{\phi^2 d}+1)^2}\,\mathrm{d}p \geqslant (2\pi)^{-3}\phi^4 \frac{1}{4}\int_{|p|\leqslant C_0} \frac{1}{p^2(p^2+1)^2}\,\mathrm{d}p = C(a)\phi^4.$$

Note that the constant $C(a)$ is independent of $d^{1/2}\phi$ in both cases. To prove the remaining assertion that $\rho_{\gamma^\delta_{\min}} \to 0$ as $d \to \infty$, use (3.44) divided by $-d\phi^2$. Note that $A^2(p) \leqslant \nu$ and, for large p, apply dominated convergence as $d \to \infty$ with the dominant $1/p^4$. For small p, the integrand is bounded due to the radial symmetry of $\widehat{Vu}$. Thus, a dominating function is obtained by choosing $d = 0$ as well. □

3.6 Proof of Theorem 1.3

The proof we give follows essentially the strategy of the proof of Theorems 10 and 11 in [3]. There, these theorems are proved simultaneously so that we give a somewhat distilled version.

Let us first explain our task. Let $\rho \geqslant 0$. Once we have found a minimizing pair $(\gamma^\delta_{\mathrm{min}}, \alpha^\delta_{\mathrm{min}})$, the number $\rho_{\gamma^\delta_{\mathrm{min}}}$ is determined uniquely. For the minimization problem (1.11), this implies that $\rho_0(\delta) = \rho - \rho_{\gamma^\delta_{\mathrm{min}}}$. Of course, all these expressions depend on δ and the remaining task to find a $\delta \geqslant 0$ such that $\rho_0(\delta)$ is sufficiently close to the minimizing ρ_0 in (1.11). This is a one-dimensional minimization problem. We shall elaborate on this problem further, so that we may carry it out explicitly in the end.

To start, let us assume that $\delta \geqslant 0$ and $\rho_0 \geqslant 0$ are such that

$$\rho = \rho_0 + \rho_{\gamma^\delta_{\mathrm{min}}}. \tag{3.46}$$

By using Lemma 3.2 we know that any minimizing triple $(\gamma, \alpha, \rho_0) \in \mathcal{D}$, which fulfills (3.4), has to satisfy

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) &\geqslant \mathcal{F}^{\mathrm{sim}}(\gamma^\delta_{\mathrm{min}}, \rho_0)\\ &= 4\pi a\rho^2 + 4\pi(a_0 - a)(\rho^2 - \rho_0^2) + \mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\mathrm{min}}, \rho_0)\end{aligned} \tag{3.47}$$

as well as

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) &\leqslant \mathcal{F}^{\mathrm{sim}}(\gamma^\delta_{\mathrm{min}}, \rho_0) + (E_1 + E_2 + E_3)(\gamma^\delta_{\mathrm{min}}, \alpha^\delta_{\mathrm{min}}, \rho_0)\\ &= 4\pi a\rho^2 + 4\pi(a_0 - a)(\rho^2 - \rho_0^2) + \mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\mathrm{min}}, \rho_0)\\ &= 4\pi a\rho^2 + 4\pi(a_0 - a)(\rho^2 - \rho_0^2) + \mathcal{O}(\rho a)^{5/2},\end{aligned} \tag{3.48}$$

where the error in (3.48) is not yet uniform in $d \geqslant 0$. Now, $\rho_{\gamma^\delta_{\mathrm{min}}}$ is decreasing in d by Lemma 3.14: $\rho_{\gamma^\delta_{\mathrm{min}}} \to 0$ as $d \to \infty$. Hence, (3.46) has a solution $\rho_0(d)$ for every ρ_0 and ρ with $\rho - \rho_{\gamma^{\delta=0}_{\mathrm{min}}} \leqslant \rho_0 \leqslant \rho$, satisfying

$$\rho - \rho_0(d) = \rho_{\gamma^\delta_{\mathrm{min}}} = (8\pi a\rho_0(d))^{3/2} I_2(\nu + d) + \mathrm{o}(\rho a)^{3/2} \tag{3.49}$$

by Theorem 3.6. Let us define

$$\mathcal{G}^\delta_\rho(\rho_0) := 4\pi(a_0 - a)(\rho^2 - \rho_0^2) + \mathcal{I}^\delta(\rho_0).$$

Lemma 3.15 (A priori estimate). *Let $\delta = 0$. There is a constant $C > 0$ such that any unconstrained minimizer $(\gamma, \alpha, \rho_0) \in \mathcal{D}$ has to satisfy*

$$\rho - \rho_0(d = 0) \leqslant C\rho^{3/2}. \tag{3.50}$$

Proof. Denote $\rho_0 = \rho_0(d = 0)$. By Theorem 3.9, there is a constant $C_0 > 0$ such that $|\mathcal{I}^0(\rho_0)| \leqslant C_0\rho_0^{5/2}$ for all sufficiently small $\rho_0 \geqslant 0$. Define $C := \frac{C_0}{2\pi(a_0 - a)}$ and assume, for contradiction, that $\rho - \rho_0 \geqslant C\rho^{3/2}$. Then, since $0 \leqslant \rho_0 \leqslant \rho$, we have

$$\begin{aligned}\mathcal{G}_\rho(\rho_0) &\geqslant 4\pi(a_0 - a)(\rho - \rho_0)\rho - C_0\rho_0^{5/2} \geqslant 4\pi(a_0 - a)C\rho^{5/2} - C_0\rho^{5/2} = (2C_0 - C_0)\rho^{5/2}\\ &= C_0\rho^{5/2} \geqslant \mathcal{I}(\rho) = \mathcal{G}_\rho(\rho).\end{aligned}$$

This implies that it is energetically favorable to minimize $\mathcal{G}_\rho(\rho_0)$ by choosing $\rho_0 = \rho$. Hence, $\rho_\gamma = 0$, contradicting the assumption $\rho_\gamma \geqslant C\rho^{3/2}$. ☐

We need to show that it suffices to consider the infimum over $d \geqslant 0$. This amounts to excluding $0 \leqslant \rho_0 \leqslant \rho_0(d=0)$ since we already know that $\rho_0(d)$ is increasing in d. To do this, we repeat the lower bound (3.47)

$$\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) \geqslant 4\pi a\rho^2 + 4\pi(a_0 - a)(\rho^2 - \rho_0^2) + \mathcal{O}(\rho a)^{5/2}$$

and see that it has a negative derivative for all $\rho_0 \geqslant 0$ so that the minimum is attained at the boundary $\rho = \rho_0$ up to a lower order error. There it matches the unconstrained lower bound (3.47), a contradiction to Lemma 3.15.

We continue by showing that it suffices to consider $d \in [0, d_0]$, for some $d_0 > 0$. To see this, use Lemma 3.14 as $d \gg 1$ to get

$$\begin{aligned}
\mathcal{F}^{\mathrm{sim}}(\gamma^\delta_{\mathrm{min}}, \rho_0) &\geqslant 4\pi a\rho^2 + \mathcal{I}^\delta(\rho_0) - d(8\pi\rho_0 a)^{3/2}\rho_{\gamma^\delta_{\mathrm{min}}} \\
&\geqslant 4\pi a\rho^2 + C(a)\min\{(\rho_0 a)^{5/2} d^{1/2}, a^{-1}(\rho_0 a)^2\} \\
&\geqslant (4\pi a + C(a))\rho^2 + C(a)\rho\rho_{\gamma^\delta_{\mathrm{min}}} + \mathcal{O}(\rho^3).
\end{aligned}$$

This is of higher order than the unconstrained upper bound (3.48). Hence, it suffices to consider $d \in [0, d_0]$, for some $d_0 > 0$, whence all errors are uniform in d due to Theorems 3.6, 3.7 and 3.9. Recall from (3.26) with $\delta = d\phi^2$ and $\phi = (8\pi a\rho_0(d))^{1/2}$ that

$$\mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\mathrm{min}}, \rho_0(d)) = (8\pi a\rho_0(d))^{5/2}\Big[I_1(\nu + d) - dI_2(\nu + d)\Big] + \mathrm{o}(\rho a)^{5/2},$$

and that

$$\rho^2 - \rho_0(d)^2 = \rho^2 - (\rho^2 - \rho_{\gamma^\delta_{\mathrm{min}}})^2 = 2\rho\rho_{\gamma^\delta_{\mathrm{min}}} + \mathrm{o}(\rho a)^{5/2}$$

according to (3.49). Plugging in (3.46), we end up with

$$\begin{aligned}
F(\rho) &= \inf_{0\leqslant d\leqslant d_0}\Big[4\pi a\rho^2 + 8\pi(a_0 - a)\rho\cdot\rho_{\gamma^\delta_{\mathrm{min}}} + \mathcal{F}^{\mathrm{s}}(\gamma^\delta_{\mathrm{min}}, \rho_0(d))\Big] + \mathrm{o}(\rho a)^{5/2} \\
&= \inf_{0\leqslant d\leqslant d_0}\Big[4\pi a\rho^2 + (8\pi a)^{5/2}(\nu - 1)\rho\rho_0(d)^{3/2} I_2(\nu + d) \\
&\qquad + (8\pi a\rho_0(d))^{5/2}\big(I_1(\nu + d) - dI_2(\nu + d)\big)\Big] + \mathrm{o}(\rho a)^{5/2} \qquad (3.51)
\end{aligned}$$

for the canonical minimization problem (1.11). Now, we would like to substitute ρ for $\rho_0(d)$ in the formula above. To do this, we perform a Taylor expansion for (3.51) in ρ_0. Recall that, by (3.49), we have $\rho - \rho_0(d) = \mathcal{O}(\rho)^{3/2}$. Consider the first term of (3.51) involving $\rho_0(d)$. Its Taylor expansion reads

$$(8\pi a)^{5/2}(\nu - 1)\rho^{5/2} I_2(\nu + d) + \frac{3}{2}(\rho_0(d) - \rho)(8\pi a)^{5/2}(\nu - 1)\rho^{3/2} I_2(\nu + d).$$

Observe that the last term is $\mathcal{O}(\rho a)^3$ and can be absorbed in the energy expansion. In the same way, we substitute $\rho_0(d)$ in the second term and obtain

$$F(\rho) = \inf_{0\leqslant d\leqslant d_0}\Big[4\pi a\rho^2 + (8\pi)^{5/2}\big(I_1(\nu + d) + (\nu - 1 - d)I_2(\nu + d)\big)(\rho a)^{5/2}\Big] + \mathrm{o}(\rho a)^{5/2}$$

We are left with performing a one-dimensional minimization problem. By considering the pointwise minimization in the integrand we get the minimum $d = \nu - 1$, whence $F(\rho)$ takes the form (1.14).

4 Conclusion and Outline

We have proved a two-term asymptotics for the homogeneous Bose gas in the thermodynamic limit. The proof used the canonical Bogolubov zero-temperature energy functional $\mathcal{F}^{\mathrm{can}}$. The minimization regime was the set of quasi-free states which, in particular, satisfy $\alpha^2 = \gamma(\gamma+1)$. We started by analyzing the simplified functional $\mathcal{F}^{\mathrm{sim}}$ which could be minimized explicitly. However, this minimization had to be constrained to the condition $\rho_0 + \rho_\gamma = \rho$ reflecting the macroscopic occupation of the ground state of the majority of the particles. An a priori estimate showed that $\rho - \rho_0 = \mathcal{O}(\rho)^{3/2}$, which means that ρ_0 is "almost all of" ρ. Using this, we could prove the lower bound. At the same time, the minimizer of $\mathcal{F}^{\mathrm{sim}}$ served as an idea for a suitable trial state with sufficiently low energy. This, in turn, proved the upper bound.

In the following, we want to compare our result to the paper [1] by Erdős, Schlein and Yau. There, the authors consider the Bose gas $H_{N,L}$ on the finite box Λ_L, compare (1.1), and construct a trial state. Afterwards, they compute its energy. The result for the energy per particle of the trial state is

$$\frac{E}{N} = 4\pi a\rho + 4\pi a\rho\left[\sqrt{\frac{32}{\pi}}\Phi(h)(a^3\rho)^{1/2}\right] + \mathrm{o}(\rho^2|\ln\rho|), \tag{4.1}$$

see [1, eq.(12)]. As mentioned in the introduction, our result carries an additional power of ρ compared to (4.1), see (1.9) and (1.14). The function Φ is given by [1, eq.(11)] and reads

$$\Phi(h) = \int_0^\infty y^{1/2}\left(\sqrt{(y+2h)(y+2+2h)} - (y+1+2h) + \frac{1}{2y}\right)\mathrm{d}y.$$

The parameter h, defined in [1, eq.(9)] is in close relation to ν, namely

$$h := \frac{\widehat{V}(0)}{8\pi a} - 1 = \nu - 1 > 0.$$

Now, a straightforward calculation shows that

$$I_1(2\nu-1) = \frac{1}{2(2\pi)^2}\Phi(h)$$

so that the second order constant of our result (1.14) reads

$$(8\pi)^{5/2} I_1(2\nu-1) = 4\pi\cdot\sqrt{\frac{32}{\pi}}\cdot\Phi(h)$$

in precise agreement with (4.1). This proves that already [1] have had the best possible upper bound among quasi-free states. Corollary 3.12 says that I_1 is strictly monotonically increasing, so that, with $\nu > 1$, our second order constant $(8\pi)^{5/2}I_1(2\nu-1)$ is strictly bigger than $(8\pi)^{5/2}I_1(1) = \frac{512\sqrt{\pi}}{15}$ in the Lee-Huang-Yang formula (1.9). Here, the value for $I_1(1)$ is given by Corollary 3.11.

Let us now understand the representation of the main theorem in [1] which we mentioned in the introduction. Applying Corollary 3.12 to I_1, we obtain

$$I_1(2\nu-1) = I_1(1) + 2\cdot I_2(1)(\nu-1) + \mathcal{O}(\nu-1)^2 \tag{4.2}$$

for small $\nu \geqslant 1$. Again, recall the values $I_1(1) = \frac{2\sqrt{2}}{15\pi^2}$ and $I_2(1) = \frac{\sqrt{2}}{12\pi^2}$ by Corollaries 3.10 and 3.11. Inserting them and (4.2) into the main result (1.14), and omitting all the error terms, we get

$$\begin{aligned} F(\rho) &\approx 4\pi a\rho^2 + \left[\frac{512\sqrt{\pi}}{15} + \frac{512\sqrt{\pi}}{12} \cdot (\nu - 1)\right](\rho a)^{5/2} \\ &= 4\pi a\rho^2 + \frac{512\sqrt{\pi}}{15}\left[1 + \frac{15}{12} \cdot (\nu - 1)\right](\rho a)^{5/2}. \end{aligned} \tag{4.3}$$

This expression has a form similar to (1.5). In [1], the authors replace the potential V by λV, with a tuning parameter $\lambda > 0$. They prove that we have the expansion $\nu - 1 = \mathcal{O}(\lambda)$ as $\lambda \to 0$, so that $\nu - 1 \leqslant C\lambda$ for a constant $C > 0$ and $\lambda > 0$ small enough. Hence, S_λ from (1.5) is equal to $1 + \frac{15}{12} \cdot C\lambda$ by the term in square brackets in (4.3).

Let us comment briefly on possible extensions to the method of this thesis. In 2009, Yau and Yin published a paper [13] in which they construct another trial state for $H_{N,L}$. Their trial state has energy precisely given by (1.4) and it has a new feature implemented. The authors call it a "soft-pair" interaction. It remains open to prove a similar lower bound for states with such soft-pair interactions. However, it is evident that the ground state of the general Bose gas has an additional feature compared to quasi-freedom that lowers the energy of second order to match (1.4). The trial state by Yau and Yin hints to the fact that this additional feature might be their soft-pair interaction: the possibility of exchange of momentum with the condensate in such a way that the total momentum is nonzero but "small". It is unknown, however, what the general definition of such states should be and what their properties are. For example, one could ask if there is an analogous property to Wick's Theorem [5, Theorem 10.2].

A first access and a somewhat different approach to treat this problem could be the ansatz to include a term into $\mathcal{F}^{\text{can}}$ of the form

$$\mu \int_{\mathbb{R}^3 \times \mathbb{R}^3} \widehat{V}(p - q)\gamma(p)\alpha(q)\,\mathrm{d}p\mathrm{d}q$$

modeling the soft-pair interaction. Here, $\mu \in \mathbb{R}$ is a tuning parameter. Then, the natural question is what the relationship between the N-body Hamiltonian and the new functional is. Nevertheless, one is inclined to try to minimize in the "same" spirit as in this thesis. We expect though that even the calculation of the minimizer of the new $\mathcal{F}^{\text{s}}$ is severly more complicated than the one given here. After all, the critical equation becomes a polynomial of degree 4 and not 2, as it is here – let alone the proofs on the way to a rigorous theorem. That conclusion is inspired by [13], where it takes more than 50 pages to construct a state and "calculate" its energy.

By now, the history of the interacting Bose gas is almost a century long. Yet, nobody understands to compute either the ground state energy or the ground state in general – let alone more involved properties. In this thesis, we worked out the ground state energy in the low-density limit for a gas with additional assumptions on the minimizing class. However, we still lack a proof of the second-order lower bound for (1.9). Concerning the existence of Bose-Einstein condensation, even less is known. Therefore, we are certain that the Bose gas will continue to challenge mathematicians and physicists in the future.

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Declaration of authorship

I declare that the work presented here is, to the best of my knowledge and belief, original and the result of my own investigations, except as acknowledged. It has not been submitted, neither in whole nor partly, for a degree at this or any other university.

Formulations and ideas taken from other sources are cited accordingly.

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