ON THE ENERGY OF DILUTE BOSE GASES

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ABSTRACT

A fundamental problem in quantum mechanics is to understand the structure and the energy of ground states of interacting systems of many particles. The quantum correlations in ground states or low lying energy states are supposed to explain phenomena such as superfluidity or superconductivity.

A long-standing conjecture in mathematical physics has been to establish a universal two-term asymptotic formula for the ground state energy of a system of bosons in the dilute limit of low density predicted by the theory of superfluidity. We discuss a recent proof of this formula.

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1. INTRODUCTION

Physical systems of many interacting particles are highly complex and extremely difficult to analyze due to the correlations between the particles.

Many-particle *quantum* systems are particularly difficult because of the added complexity caused by entanglement leading to quantum correlations. Exotic phenomena such as superfluidity and superconductivity are due to such quantum correlations. We are still very far from being able to give a full mathematical explanation of these phenomena, but recent years have seen some progress on these very fundamental issues.

We will give a short account of progress on a particularly fundamental aspect of the analysis of quantum many-particle systems. The question is to understand the ground state, i.e., the state of lowest energy, of an interacting quantum system of identical particles in three dimensions. Consider a large, i.e., thermodynamic, system of density $\rho > 0$ of identical nonrelativistic particles. The only assumption we make about the interaction between these particles is that it is a repulsive two-body interaction. The question is what is the ground state energy density of such a system. In a seminal paper from 1957 [12], Lee, Huang, and Yang predicted that there is a universal asymptotic formula for the energy density $e(\rho)$ in the dilute limit given by

$$e(\rho) = (\hbar^2/2m)4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho a^3})\right). \tag{1.1}$$

The formula is referred to as universal because there is a two-term asymptotic expansion depending on the interaction potential through only one parameter, *the scattering length* a. We will define it below. Above $\hbar$ is Planck's constant and m is the mass of the particles. The diluteness of the system is measured in terms of the dimensionless parameter ρa^3, i.e., the expected number of particles in a cube of size a. In [12] the prediction was based on a heuristic analysis of the case of a hard core potential of radius a, i.e., particles move freely except that they cannot get closer than a distance a from each other. Formula (1.1) can also be understood heuristically from Bogolubov's theory of superfluidity from 1947 [4]. We will describe a recent proof [8, 9] that establishes the formula for a very large class of repulsive interaction potentials. The Lee–Huang–Yang formula has been tested experimentally on a gas of ^{7}Li atoms in [18]. Here the coefficient which in the formula is $\frac{128}{15\sqrt{\pi}} = 4.81$ was measured to be 4.5 ± 0.7 in excellent agreement with the theoretical value.

This paper is organized as follows. In Section 2 we explain the mathematical formulation of many-particle quantum systems with two-body interactions. We, in particular, introduce the thermodynamic limit of the ground state energy density for translation-invariant systems. In Section 3 we consider the simple case of just two particles and use it to introduce the scattering length and give the precise statements of the main theorems. In Section 4 we briefly introduce the second quantized formalism and give the heuristics behind Bogolubov's approximation that leads to his theory of superfluidity for weakly interacting Bose gases. We will also explain how the Lee–Huang–Yang (LHY) formula can be heuristically derived from the Bogolubov approximation. In Section 5 we sketch the ingredients of the rigorous proof of the LHY formula. The details of what is being discussed here can be found in [8, 9].

2. QUANTUM MANY-PARTICLE HAMILTONIANS WITH 2-BODY INTERACTIONS

We consider N identical particles moving in a box $\Omega = [0, L^3]$ described by the basic two-body Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le i < j \le N} V(x_i - x_j) \tag{2.1}$$

acting as a self-adjoint operator on an appropriate domain on $\mathcal{H}_N = L^2(\Omega^N) = \bigotimes^N L^2(\Omega)$. We have chosen units such that $\hbar = 2m = 1$, where m is the mass of the particles. The first sum in the Hamiltonian describes the kinetic energy of the nonrelativistic particles. For simplicity, we may assume that we have periodic boundary conditions such that Ω represents a torus, but, as we shall see, this is not really important. In the periodic case we see that the Hamiltonian above is translation invariant. The second sum in the Hamiltonian is the interaction. The only assumption we make about the interaction potential V is that it is repulsive, i.e., it could be any measurable function $V : \mathbb{R}^3 \to [0, \infty]$, spherically symmetric, and has suffient decay. For simplicity, we will here assume that it has compact support, but this can be relaxed considerably (see [9]).

A particularly interesting example is the hard core potential

$$V(x) = \begin{cases} 0, & |x| > a, \\ \infty, & |x| \le a. \end{cases} \tag{2.2}$$

Since the Hamiltonian is symmetric under interchange of particles, it could also be restricted to the fully symmetric subspace $\mathcal{H}_N^{\mathrm{B}} = \bigvee^N L^2(\Omega)$ or the fully antisymmetric subspace $\mathcal{H}_N^{\mathrm{F}} = \bigwedge^N L^2(\Omega)$. In the first case we describe bosons, while in the second case we describe fermions.

The spectrum of the operator H_N will be discrete. The lowest eigenvalue is referred to as the *ground state energy*

$$E(N, \Omega, V) = \inf \mathrm{Spec}_{\mathcal{H}_N} H_N = \inf \mathrm{Spec}_{\mathcal{H}_N^{\mathrm{B}}} H_N. \tag{2.3}$$

Note that for the ground state energy it does not play any role whether we consider the full space $\mathcal{H}_N$ or the bosonic subspace $\mathcal{H}_N^{\mathrm{B}}$: By a classical theorem, the ground state eigenvector will be symmetric. As physical particles are either bosons or fermions, we refer to our analysis as the ground state of a Bose gas, but from a mathematical point of view this restriction is not important. Nevertheless, we shall in Section 4.1 use the second quantized techniques developed particularly for Bose gases.

The important quantity that we will analyze is the thermodynamic limit of the ground state energy density

$$e(\rho, V) = \lim_{L \to \infty, N/L^3 = \rho} L^{-3} E(N, \Omega, V), \tag{2.4}$$

where we have fixed the density of particles to be $\rho \ge 0$. It is not difficult to see that the limit in (2.4) exists and it is indeed independent on the type of boundary condition that was

chosen for the Hamiltonian. An alternative formulation would be not to fix the density but to introduce a chemical potential μ and define

$$e_{\mathrm{gc}}(\mu, V) = \lim_{L\to\infty,} L^{-3} \inf_{N\geq 0} \big(E(N, \Omega, V) - \mu N\big). \tag{2.5}$$

This is referred to as the grand canonical (gc) formalism. The two "energy densities" are related by a Legendre transform

$$e(\rho, V) = \sup_{\mu} \big(e_{\mathrm{gc}}(\mu, V) + \mu\rho\big). \tag{2.6}$$

3. THE 2-PARTICLE CASE AND THE SCATTERING LENGTH

In the case that we have only two particles $N = 2$ there exists a length a, called the *scattering length* such that

$$E(2, \Omega, V) = 8\pi a L^{-3}\big(1 + O(a/L)\big). \tag{3.1}$$

The problem can be studied by analyzing the simple Schrödinger operator $-\Delta + \frac{1}{2}V$ on $L^2(\mathbb{R}^3)$. Indeed, we introduce the *scattering solution*, i.e., the unique function $\varphi : \mathbb{R}^3 \to [0, \infty)$ satisfying the zero energy equation

$$\left(-\Delta + \frac{1}{2}V\right)\varphi = 0$$

with the limiting condition $\lim_{x\to\infty} \varphi = 1$. Then, in terms of the scattering length, the scattering solution satisfies $\varphi(x) = 1 - a/|x|$ for x outside a ball containing the support of V. Moreover,

$$\int V\varphi = 8\pi a.$$

Since we also have $0 \leq \varphi \leq 1$, we see that $8\pi a \leq \int V$. In the case of the hard core (2.2), the scattering length is indeed the radius a of the core. In this case $\int V = \infty$, whereas the scattering length is finite.

We are now in a position to state the main result on the Lee–Huang–Yang asymptotics. The asymptotic formula is proved by giving upper and lower bounds for the energy density $e(\rho, V)$. The upper bound is proved by constructing approximate trial ground state eigenfunctions that reproduce the asymptotics. Establishing a matching lower bound is usually considered more difficult as it requires ideas of how to control unimportant parts of the Hamiltonian. The upper bound has, however, proved to be very difficult too, and today the lower bound requires fewer assumptions on the potential than the upper bound.

The main results on the upper and lower bounds establishing the LHY formula are given in the next two theorems.

Theorem 3.1 (The lower bound in the LHY formula). *If $V : \mathbb{R}^3 \to [0, \infty]$ is measurable, spherically symmetric with compact support then there exist a constant $C > 0$, depending only on the support of V, and an explicit number $\eta > 0$ such that*

$$e(\rho) \geq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} - C(\rho a^3)^{\frac{1}{2}+\eta}\right). \tag{3.2}$$

This lower bound was established in [8, 9].

Theorem 3.2 (The upper bound in the LHY formula). *If* $0 \leq V \in L^3(\mathbb{R}^3)$*, spherically symmetric with compact support then there exists a constant* $C > 0$ *depending on the potential* V *such that*

$$e(\rho) \leq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + C(\rho a^3)^{\frac{1}{2}+\frac{1}{10}}\right). \tag{3.3}$$

The upper bound as stated here was proved in [1]. The first proof of an upper bound giving the first two terms was established in [19].

It is not difficult to heuristically understand the leading term as we shall now explain. In the dilute limit, it is natural to expect to find the energy to be the energy of two particles times the number of pairs. This would then, indeed, lead to an approximation for $e(\rho, V)$ given by

$$\lim_{L\to\infty, N/L^3=\rho} L^{-3}\frac{N(N-1)}{2}E(2, \Omega, V) = 4\pi\rho^2 a.$$

It is, however, already difficult to get an upper bound that reproduces this correctly. To illustrate this difficulty, notice that the simple constant trial state

$$\Psi_L = L^{-3N/2} \tag{3.4}$$

that minimizes the kinetic energy gives

$$\lim_{L\to\infty, N/L=\rho} L^{-3}\langle \Psi_L, H_N \Psi_L\rangle = \frac{1}{2}\rho^2 \int V$$

which, as we saw above, can be much bigger than $4\pi\rho^2 a$. The main difficulty is to understand how to improve the large value $\int V$ with the smaller scattering length expression $8\pi a$.

We end this section by giving a short review of the history of the formula which has been a major open problem in mathematical physics for over 60 years. Additional details can be found in [14]. The leading term in the LHY expansion (1.1) was predicted by Lenz in [13]. The first to analyze it rigorously was Freeman Dyson in [6], i.e., in the same volume of Physical Review in which the paper of Lee, Huang, and Yang appeared. Dyson, indeed, proved an upper bound which gave the correct leading term for the hard sphere gas. In the case of the hard sphere gas, Dyson's upper bound still today gives the best known error term of order $(\rho a^3)^{1/3}$, which is unfortunately not of the LHY order. Dyson also gave a lower bound of the right leading order, but with a wrong constant. It took another 40 years before Lieb and Yngvason in [17] established the lower bound with the correct constant. Ten years later Erdős, Schlein, and Yau noticed in [7] that the Gaussian or quasi-free states in Bogolubov's theory of superconductivity can be used to give an upper bound that is correct to leading order and has an error term of the same order as the second term in the LHY formula but with a wrong constant. Later Yau and Yin [19] improved on the quasi-free states to get the correct LHY formula as an upper bound. Both [7] and [19] require some regularity of the potential and do not work for the hard core. In [5, 10] the correct second term in the LHY formula was derived for sufficiently soft potentials, i.e., potentials that were allowed to depend in particular ways on the diluteness parameter. Finally, the correct LHY lower bound

was proved first for general L^1 potentials in [8] and then in the most general case stated above in [9]. For gases confined to boxes of size $(\rho a)^{-1/2}$, the LHY formula was derived in [2,3]. The length scale $(\rho a)^{-1/2}$ is called the *healing length* and its relevance will become clear when we discuss Bogolubov's theory in the next section.

4. BOGOLUBOV'S THEORY OF SUPERFLUIDITY

The LHY formula for the ground state energy can heuristically be understood from Bogoliubov's theory of superfluidity [4]. Thus in some sense establishing the LHY formula validates Bogolubov's theory. We will briefly describe this here, but it will require us to take a little detour into the second quantized formalism.

4.1. Second quantized formalism

For any function $f \in L^2(\Omega)$, we introduce the bosonic *annihilation operator*

$$a(f) : \mathcal{H}_N^{\mathrm{B}} \to \mathcal{H}_{N-1}^{\mathrm{B}}$$

defined by

$$\big(a(f)\Psi\big)(x_1, \dots, x_{N-1}) = \sqrt{N} \int_\Omega \overline{f(x_N)} \Psi(x_1, \dots, x_{N-1}, x_N)\, dx_N.$$

The bosonic *creation operator* $a^\dagger(f) : \mathcal{H}_{N-1}^{\mathrm{B}} \to \mathcal{H}_N^{\mathrm{B}}$ is the adjoint $a^\dagger(f) = a(f)^*$ of $a(f)$. We here use the standard notation in physics to indicate the adjoint with a †. We deliberately did not put a subscript N on the creation or annihilation operators because we want to use the same notation independently of N. Indeed, this will allow us to write the famous commutation relations

$$\big[a(f), a(g)\big] = 0, \quad \big[a(f), a^\dagger(g)\big] = (g, f)_{L^2(\Omega)}.$$

Using the second quantization formalism, we can rewrite the Hamiltonian H_N (at least for L large enough) as

$$\begin{aligned} H &= \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} p^2 a_p^\dagger a_p + \frac{1}{2L^3} \sum_{p,q,k \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{V}(k) a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p \\ &= \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} p^2 a_p^\dagger a_p + \frac{N-1}{2} \rho \hat{V}(0) + \frac{1}{2L^3} \sum_{0 \neq k \in \frac{2\pi}{L}\mathbb{Z}^3} \sum_{p,q \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{V}(k) a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p, \end{aligned} \tag{4.1}$$

where we used the short hand notation $a_p = a(L^{-3/2} \exp(ipx))$. These operators satisfy the commutation relations

$$\big[a_p, a_q\big] = 0, \quad \big[a_p, a_q^\dagger\big] = \delta_{p,q}. \tag{4.2}$$

We have also introduced the Fourier transform

$$\hat{V}(k) = \int_{\mathbb{R}^3} \exp(-ipx) V(x) dx.$$

4.2. The Bogolubov's approximation

In his 1947 paper [4], Bogolubov introduces an approximation to the Hamiltonian H_N, or in fact to the operator H in (4.1), that forms the basis of his theory of superfluidity. Bogolubov's approximation may be divided into three steps.

Step 1. Condensation and c-number substitution. The assumption is that the ground state or low lying energy states represent a condensate, i.e., have many particles with momentum $p = 0$. If all particles had momentum $p = 0$, we would get the state (3.4) which we know does not have the correct ground state energy. It is, however, still possible that the expectation of the operator $a_0^\dagger a_0$ in the ground state is close to the total number of particles N. The second ingredient in this first step of the approximation is to replace the operators a_0 and $a_0^\dagger$ by the number $\sqrt{N}$ in the Hamiltonian H in (4.1). This is referred to as c-number substitution. It will lead to an operator that no longer maps $\mathcal{H}_N^{\mathrm{B}}$ to itself. We consider it instead as an operator on the *bosonic Fock space* $\bigoplus_{M=0}^{\infty} \mathcal{H}_M^{\mathrm{B}}$.

Step 2. The Bogolubov's Hamiltonian. The first step results in a Hamiltonian that will have terms containing zero, two, three, or four factors $a_p^\dagger$ or a_p with $p \neq 0$. There are no terms with only one $a_p^\dagger$ or a_p with $p \neq 0$ because of momentum conservation. The second step in the approximation is to assume that we may consider $a_p^\dagger$ or a_p with $p \neq 0$ to be small and therefore ignore terms with three or more such factors. This will lead to the Bogolubov's Hamiltonian

$$H_{\mathrm{Bog}} = \sum_{0 \neq p \in \frac{2\pi}{L}\mathbb{Z}^3} \left(\big(p^2 + \rho \hat{V}(p)\big) a_p^\dagger a_p + \frac{1}{2}\rho \hat{V}(p)\big(a_p^\dagger a_{-p}^\dagger + a_{-p} a_p\big) \right) + \frac{N-1}{2}\rho \hat{V}(0). \tag{4.3}$$

Step 3. Diagonalizing the Bogolubov's Hamiltonian. It is not difficult to diagonalize the Bogolubov's Hamiltonian if we apply the following simple lemma whose proof is elementary.

Lemma 4.1 (Simple case of Bogoliubov's diagonalization). *For $\mathcal{A} > 0$, $\mathcal{B} \in \mathbb{R}$ satisfying $|\mathcal{B}| \leq \mathcal{A}$, we have the operator identity*

$$\mathcal{A}(a_p^\dagger a_p + a_{-p}^\dagger a_{-p}) + \mathcal{B}(a_p^\dagger a_{-p}^\dagger + a_{-p} a_p) = \mathcal{D}(b_p^\dagger b_p + b_{-p}^\dagger b_{-p}) - (\mathcal{A} - \sqrt{\mathcal{A}^2 - \mathcal{B}^2}), \tag{4.4}$$

where

$$\mathcal{D} := \sqrt{\mathcal{A}^2 - \mathcal{B}^2}, \tag{4.5}$$

and

$$b_p := (1-\alpha^2)^{-1/2}(a_p + \alpha a_{-p}^\dagger), \quad b_{-p} := (1-\alpha^2)^{-1/2}(a_{-p} + \alpha a_p^\dagger), \tag{4.6}$$

with

$$\alpha := \mathcal{B}^{-1}(\mathcal{A} - \sqrt{\mathcal{A}^2 - \mathcal{B}^2}). \tag{4.7}$$

Note that the operators b_p and $b_p^\dagger$ satisfy the same commutation relations (4.2) as the operators a_p and $a_p^\dagger$. We see that the Bogolubov's Hamiltonian may be rewritten as

$$H_{\text{Bog}} = \left(\sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \varepsilon(p) b_p^\dagger b_p \right) + E_L \tag{4.8}$$

with

$$\varepsilon(p) = \sqrt{\left(p^2 + \rho\hat{V}(p)\right)^2 - \left(\rho\hat{V}(p)\right)^2}), \tag{4.9}$$

and where the ground state energy of H_{Bog} is

$$E_L = \frac{N-1}{2}\rho\hat{V}(0) - \frac{1}{2} \sum_{0 \neq p \in \frac{2\pi}{L}\mathbb{Z}^3} \left(\left(p^2 + \rho\hat{V}(p)\right) - \sqrt{\left(p^2 + \rho\hat{V}(p)\right)^2 - \left(\rho\hat{V}(p)\right)^2}\right). \tag{4.10}$$

The ground state of the Bogolubov's Hamiltonian is the vacuum state for the operators b_p. Such vacuum states of general bosonic annihilation operators are referred to as (pure) quasi-free or Gaussian states.

In the thermodynamic limit, we have $\lim_{L\to\infty, N/L^3=\rho} \frac{E_L}{L^3} = e_{\text{Bog}}(\rho, V)$, where

$$\begin{aligned} e_{\text{Bog}}(\rho, V) = \frac{1}{2}\rho^2 \int V \\ - \frac{1}{2}(2\pi)^{-3} \int_{\mathbb{R}^3} \left(\left(p^2 + \rho\hat{V}(p)\right) - \sqrt{\left(p^2 + \rho\hat{V}(p)\right)^2 - \left(\rho\hat{V}(p)\right)^2}\right) dp. \end{aligned} \tag{4.11}$$

We may rewrite this as

$$\begin{aligned} e_{\text{Bog}}(\rho, V) = 4\pi\rho^2(a_0 + a_1) \\ - \frac{1}{16\pi^3} \int p^2 + \rho\hat{V}(p) - \sqrt{p^4 + 2\rho\hat{V}(p)p^2} - \rho^2 \frac{\hat{V}(p)^2}{2p^2}\, dp, \end{aligned} \tag{4.12}$$

where we have introduced the notation

$$a_0 = \frac{1}{8\pi}\int V, \quad a_1 = \frac{-1}{(8\pi)^2} \iint \frac{V(x)V(y)}{|x-y|}\, dxdy = \frac{-1}{64\pi^4} \int \frac{\hat{V}(p)^2}{2p^2}\, dp. \tag{4.13}$$

In fact, a_0 and a_1 are the first two terms in what is called the *Born series* for the scattering length a. In the last integral in (4.12), we can change variable $p = \sqrt{8\pi\rho a_0}q$ and arrive at

$$\begin{aligned} \int p^2 + \rho\hat{V}(p) - \sqrt{p^4 + 2\rho\hat{V}(p)p^2} - \rho^2 \frac{\hat{V}(p)^2}{2p^2}\, dp \\ = (8\pi\rho a_0)^{5/2} \int q^2 + W_\rho(q) - \sqrt{q^4 + 2W_\rho(q)q^2} - \frac{W_\rho(q)^2}{2q^2}\, dq, \end{aligned} \tag{4.14}$$

where we wrote $W_\rho(q) = (8\pi a_0)^{-1}\hat{V}(\sqrt{8\pi\rho a_0}q)$. In the dilute limit, we may assume that $(\rho a_0)^{-1/2}$ is much longer than the range of the potential and hence we can, to leading order in the integral, replace $W_\rho(q)$ by $W_\rho(0) = 1$. Since

$$\int_{\mathbb{R}^3} q^2 + 1 - \sqrt{q^4 + 2q^2} - \frac{1}{2q^2}\, dq = -\frac{32\sqrt{2}\pi}{15},$$

we arrive at

$$e_{\mathrm{Bog}}(\rho, V) \approx 4\pi\rho^2(a_0 + a_1) + 4\pi\rho^2 a_0 \frac{128}{15\sqrt{\pi}} \sqrt{\rho a_0^3}. \tag{4.15}$$

If we replace the first two Born terms $a_0 + a_1$ by the scattering length a in the first term and a_0 by a in the second term above, we arrive at the Lee–Huang–Yang formula. We note that the change of variable $p = \sqrt{8\pi\rho a_0} q$ in the integral above shows that the relevant momenta that contribute to the LHY formula are of order of the inverse healing length $\sqrt{\rho a}$.

Understanding the validity of the Bogolubov's approximation and the validity of these last replacements above were the major challenges in establishing the LHY formula rigorously. We address this in the next section. We will end this section with a few further remarks about the Bogolubov's approximation and Bogolubov's theory of superfluidity.

In his treatment [11] of superfluidity in helium, Landau realized the importance of a linear dispersion law, i.e., that the energies of excitations grow linearly with momentum. The slope in the linear dispersion represents the critical velocity for superfluidity, i.e., the velocity below which objects can move through the fluid without creating excitations. We see that the dispersion $\varepsilon(p)$ in (4.9), indeed, has a nonvanishing linear slope $\lim_{p\to 0} |\nabla\varepsilon(p)| = \sqrt{2\rho\hat{V}(0)}$. This is the central point in Bogolubov's theory of superfluidity in weakly interacting Bose gases.

5. RIGOROUS PROOF OF THE LEE–HUANG–YANG FORMULA

In this section we very briefly sketch the rigorous arguments, leading to the lower bound in Theorem 3.1. The details can be found in [8, 9].

An important ingredient in the Bogolubov's approximation was the assumption of condensation. It is still a great mathematical challenge to establish Bose condensation in nontrapped translation invariant Bose gases. To circumvent this, the first step in the rigorous derivation of the Lee–Huang–Yang formula in [8, 9] is a localization to boxes that are essentially of the order of the healing length. On this scale, it turns out that the gas will look sufficiently condensed. In other words, it is not possible to show that most particles in a thermodynamic box are in a state of momentum zero. We can, however, show that most particles have momenta small compared to the inverse healing length.

For the rigorous lower bound, the localization is achieved by an operator estimate on the Hamiltonian

$$H_N - \mu N \geq \int h_u \, du, \tag{5.1}$$

where we introduced the chemical potential μ that we will write $\mu = 8\pi\rho_\mu a$. The reason for this choice is that if we insert the leading term in the LHY formula $4\pi\rho^2 a$ for the energy density then the choice of ρ that minimizes $4\pi\rho^2 a - \mu\rho = 4\pi\rho^2 a - 8\pi\rho_\mu a\rho$ is indeed $\rho = \rho_\mu$. The operators h_u above represent translations by $u \in \mathbb{R}^3$ of a Hamiltonian h_0 localized to a box $[0, \ell]^3$ with length $\ell = K_\ell(\rho_\mu a)^{-1/2}$ for a sufficiently large constant K_ℓ, i.e., we are localizing on scales that are large compared to the healing length.

To describe the localized Hamiltonian h_0, we introduce the orthogonal projection P that projects onto the one-dimensional space of constant functions in $L^2([0,\ell]^3)$ and the projection $Q = I - P$ onto the orthogonal complement. We also introduce a sufficiently regular function $\chi : \mathbb{R}^3 \to [0,\infty)$ supported on $[0,1]^3$ and let $\chi_\ell(x) = \chi(x/\ell)$.

The localized Hamiltonian then has the form

$$h_0 = \sum_{i=1}^{N} T_i - \rho_\mu \sum_{i=1}^{N} \int w_1(x_i, y)dy + \sum_{1\le i<j\le N} w(x_i, x_j), \tag{5.2}$$

where the localized kinetic energy is

$$T = Q\chi_\ell K(\Delta)\chi_\ell Q + QG_0Q \tag{5.3}$$

with $K(t)$ being a function that is essentially the identity for $t \gg \ell^{-2}$ and G_0 an operator that ensures a sufficient gap above zero in the kinetic energy, i.e., an important property is $G_0 \ge (\text{const})\ell^{-2}$. The exact forms of K and G_0 are complicated and can be found in [8,9]. The potential function is

$$w(x,y) = \chi_\ell(x)\frac{V(x-y)}{\chi * \chi(x/\ell)}\chi_\ell(y), \quad w_1(x,y) = w(x,y)\varphi(x-y), \tag{5.4}$$

where we recall that φ is the scattering solution. For the potential part of the Hamiltonian, it is not difficult to see that (5.1) is actually an identity. It is for the kinetic energy that it becomes a lower bound.

In order to establish condensation, it is necessary to obtain an a priori lower bound on the ground state energy of h_0 of the correct LHY order. This is achieved in [8,9] by doing a further localization that we shall not discuss here. Such an a priori lower bound establishes a bound on the expectation of the number of noncondensed particles $n_+ = \sum_{i=1}^{N} Q_i$. Indeed, the bound on the gap operator G_0 and the a priori bound imply that any state that does not already satisfy an LHY lower bound would have

$$(\text{const})\ell^{-2}\langle n_+\rangle \le \langle G_0\rangle \le \rho_\mu^2 a\sqrt{\rho_\mu a^3}\ell^3,$$

i.e., $\langle n_+\rangle \le C\rho_\mu^2 a\ell^5 = K_\ell^2\sqrt{\rho_\mu a^3}\rho_\mu\ell^3$. In other words, the expected number of noncondensed particles is smaller by the (small) factor $K_\ell^2\sqrt{\rho_\mu a^3}$ compared to the expected number of particles $\rho_\mu\ell^3$ in the box. Unfortunately, it is not sufficient to control the *expected* number of noncondensed particles. There are terms that require controlling powers of the number of noncondensed particles. To achieve control of powers, we establish in [8] a stronger version of condensation, namely that it is enough to restrict attention to the part of the Hilbert space where we have the operator bound $n_+ \le \mathcal{M}$ for some appropriately chosen parameter $\mathcal{M}$. Unfortunately, in order to treat the hard core potential, in [9] we had to work with a much more complicated restriction, namely that $n_+^I \le \mathcal{M}_I$ where n_+^I represents the number of particles with kinetic energy in an interval $I = (0, K_I\ell^{-2})$, for an appropriately large constant K_I. This means $n_+^I = \sum_{i=1}^{N} \mathbb{1}_I(T)_i$. Note that n_+^I would be equal to n_+ if $K_I = \infty$. The point is that only restricting this operator allows us to choose a much smaller $\mathcal{M}_I$ than we would if we had to restrict n_+. The argument required to restrict the Hilbert space uses a method developed in [16] referred to as localization of large matrices.

Having established control on the number of noncondensed particles we use c-number substitution to treat the condensed particles. This can be done rigorously using the method in [15].

A very central point in our analysis is a decomposition of the localized interaction potential using in a very particular way the scattering solution φ. As $0 \leq \varphi \leq 1$, it is convenient to introduce the function $\omega = 1 - \varphi$ satisfying $0 \leq \omega \leq 1$ and tending to zero at infinity. The following decomposition is an elementary, but crucial, identity from [8]:

$$-\rho_\mu \sum_{i=1}^{N} \int w_1(x_i, y)\, dy + \sum_{1 \leq i < j \leq N} w(x_i, x_j) = \mathcal{Q}_0^{\mathrm{ren}} + \mathcal{Q}_1^{\mathrm{ren}} + \mathcal{Q}_2^{\mathrm{ren}} + \mathcal{Q}_3^{\mathrm{ren}} + \mathcal{Q}_4^{\mathrm{ren}},$$

where

$$\begin{aligned}
\mathcal{Q}_4^{\mathrm{ren}} &:= \frac{1}{2} \sum_{i \neq j} \big[Q_i Q_j + (P_i P_j + P_i Q_j + Q_i P_j) \omega(x_i - x_j) \big] w(x_i, x_j) \\
&\qquad \times \big[Q_j Q_i + \omega(x_i - x_j)(P_j P_i + P_j Q_i + Q_j P_i) \big], \\
\mathcal{Q}_3^{\mathrm{ren}} &:= \sum_{i \neq j} P_i Q_j w_1(x_i, x_j) Q_j Q_i + h.c., \\
\mathcal{Q}_2^{\mathrm{ren}} &:= \sum_{i \neq j} P_i Q_j w_2(x_i, x_j) P_j Q_i + \sum_{i \neq j} P_i Q_j w_2(x_i, x_j) Q_j P_i \\
&\qquad - \rho_\mu \sum_{i=1}^{N} Q_i \int w_1(x_i, y)\, dy Q_i + \frac{1}{2} \sum_{i \neq j} \big(P_i P_j w_1(x_i, x_j) Q_j Q_i + h.c. \big), \\
\mathcal{Q}_1^{\mathrm{ren}} &:= \sum_{i,j} P_j Q_i w_2(x_i, x_j) P_i P_j - \rho_\mu \sum_i Q_i \int w_1(x_i, y)\, dy P_i + h.c., \\
\mathcal{Q}_0^{\mathrm{ren}} &:= \frac{1}{2} \sum_{i \neq j} P_i P_j w_2(x_i, x_j) P_j P_i - \rho_\mu \sum_i P_i \int w_1(x_i, y)\, dy P_i.
\end{aligned}$$

Here $w_2(x, y) = w_1(x, y)(1 + \omega(x, y))$. The main observation is that the term $\mathcal{Q}_4^{\mathrm{ren}}$ is nonnegative and can be ignored for a lower bound. We think of the terms with zero to four Q's as being similar to the corresponding terms in the Bogolubov's analysis with zero to four factors of a_p or $a_p^\dagger$ with $p \neq 0$. Note that in ignoring the term $\mathcal{Q}_4^{\mathrm{ren}}$ we are not simply ignoring the term with four Q's as Bogolubov did.

The term $\mathcal{Q}_2^{\mathrm{ren}}$, together with the kinetic energy, can be rewritten in a form similar to a Bogolubov's Hamiltonian and can be diagonalized using a Bogolubov-type diagonalization argument. Note that $\mathcal{Q}_2^{\mathrm{ren}}$ contains the potentials w_1 and w_2. The potential w_1 is a localization of $V\varphi$ that satisfies $\widehat{V\varphi}(0) = 8\pi a$. This is the reason that our analysis will immediately lead to the scattering length appearing and not only the Born approximations a_0 and $a_0 + a_1$.

The appearance of w_2 in $\mathcal{Q}_2^{\mathrm{ren}}$ means that the analysis of the $\mathcal{Q}_2^{\mathrm{ren}}$ does not directly give the LHY formula. The additional contributions from the difference between w_1 and w_2 will, however, be exactly canceled by a careful analysis of the term $\mathcal{Q}_3^{\mathrm{ren}}$. This term can again be approximately diagonalized, this time together with the excitation Hamiltonian from the Bogolubov's diagonalization, i.e., the analog of the first term in (4.8). This, however, first requires estimating the operator PQw_1QQ appearing in $\mathcal{Q}_3^{\mathrm{ren}}$ in terms of an operator

$PQ_L w_1 Q_H Q_H$ where Q_L essentially projects onto appropriately low (but still nonzero) momenta and Q_H projects onto high momenta disjoint from the low momenta. Note that the operator $PQ_L w_1 Q_H Q_H$ is quadratic in Q_H which is why it allows for a Bogolubov's treatment similar to the treatment of $\mathcal{Q}_2^{\mathrm{ren}}$.

In Bogolubov's case there was no term corresponding to $\mathcal{Q}_1^{\mathrm{ren}}$ because of momentum conservation. Here our spatial localization breaks momentum conservation, and we therefore have a term $\mathcal{Q}_1^{\mathrm{ren}}$. This term can fairly easily be treated together with the $\mathcal{Q}_2^{\mathrm{ren}}$ term in the first Bogolubov's diagonalization.

Putting these ingredients together is rather technical but eventually leads to the rigorous lower bound in Theorem 3.1.

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