THE GROUND STATE OF THE BOSE GAS

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Abstract. Now that the low temperature properties of quantum-mechanical many-body systems (bosons) at low density, ρ, can be examined experimentally it is appropriate to revisit some of the formulas deduced by many authors 4-5 decades ago. For systems with repulsive (i.e. positive) interaction potentials the experimental low temperature state and the ground state are effectively synonymous – and this fact is used in all modeling. In such cases, the leading term in the energy/particle is $2\pi\hbar^2 a\rho/m$ where a is the scattering length of the two-body potential. Owing to the delicate and peculiar nature of bosonic correlations (such as the strange $N^{7/5}$ law for charged bosons), four decades of research failed to establish this plausible formula rigorously. The only previous lower bound for the energy was found by Dyson in 1957, but it was 14 times too small. The correct asymptotic formula has recently been obtained by us and this work will be presented. The reason behind the mathematical difficulties will be emphasized. A different formula, postulated as late as 1971 by Schick, holds in two-dimensions and this, too, will be shown to be correct. With the aid of the methodology developed to prove the lower bound for the homogeneous gas, two other problems have been successfully addressed. One is the proof by us that the Gross-Pitaevskii equation correctly describes the ground state in the 'traps' actually used in the experiments. For this system it is also possible to prove complete Bose condensation, as we have shown. Another topic is a proof that Foldy's 1961 theory of a high density Bose gas of charged particles correctly describes its ground state energy. All of this is quite recent work and it is hoped that the mathematical methodology might be useful, ultimately, to solve more complex problems connected with these interesting systems.

Foreword

At the conference "Contemporary Developments in Mathematics", hosted by the MIT and Harvard University Mathematics Departments, November 16–17, 2001, one of us (E.H.L.) contributed a talk with the title "The Bose gas: A subtle many-body problem". This talk covered material by all the authors listed above. This contribution is a much expanded version of the talk and of [L3].

Contents

1. Introduction

Schrödinger's equation of 1926 defined a new mechanics whose Hamiltonian is based on classical mechanics, but whose consequences are sometimes non-intuitive from the classical point of view. One of the most extreme cases is the behavior of the ground (= lowest energy) state of a many-body system of particles. Since the ground state function $\Psi(\vec{x}_1, ..., \vec{x}_N)$ is automatically symmetric in the coordinates $\vec{x}_j \in \mathbb{R}^3$ of the N particles, we are dealing necessarily with *'bosons'.* If we imposed the Pauli exclusion principle (antisymmetry) instead, appropriate for electrons, the outcome would look much more natural and, oddly, more classical. Indeed, the Pauli principle is *essential* for understanding the stability of the ordinary matter that surrounds us.

Recent experiments have confirmed some of the bizarre properties of bosons close to their ground state, but the theoretical ideas go back to the 1940's – 1960's. The first sophisticated analysis of a gas or liquid of *interacting* bosons is due to Bogolubov in 1947. His approximate theory as amplified by others, is supposed to be exact in certain limiting cases, and some of those cases have now been verified rigorously (for the ground state energy) — 3 or 4 decades after they were proposed.

The discussion will center around four main topics.

1. The dilute, homogeneous Bose gas with repulsive interaction (2D and 3D).
2. Repulsive bosons in a trap (as used in recent experiments) and the 'Gross-Pitaevskii' equation.
3. Bose-Einstein condensation for dilute trapped gases.

4. Foldy's 'jellium' model of charged particles in a neutralizing background.

Note that for potentials that tend to zero at infinity 'repulsive' and 'positive' are synonymous — in the quantum mechanical literature at least. In classical mechanics, in contrast, a potential that is positive but not monotonically decreasing is not called repulsive.

The discussion below of topic 1 is based on [LY1] and [LY2], and of topic 2 on [LSeY1] and [LSeY2]. See also [LY3, LSeY3, Se2, LSeY4]. The discussion of topic 3 is mainly taken from [LSe], but for transparency we also include here a section on the special case when the trap is a rectangular box. This case already contains the salient points, but avoids several complications due the the inhomogeneity of the gas in a general trap. The discussion of topic 4 is based on [LSo].

Topic 1 (3-dimensions) was the starting point and contains essential ideas. It is explained here in some detail and is taken, with minor modifications (and corrections), from [LY3]. In terms of technical complexity, however, the fourth topic is the most involved and can not be treated here in full detail.

The interaction potential between pairs of particles in the Jellium model in topic 4 is the repulsive, *long-range* Coulomb potential, while in topics 1–3 it is assumed to be repulsive and *short range*. For alkali atoms in the recent experiments on Bose Einstein condensation the interaction potential has a repulsive hard core, but also a quite deep attractive contribution of van der Waals type and there are many two body bound states [PS]. The Bose condensate seen in the experiments is thus not the true ground state (which would be a solid) but a metastable state. Nevertheless, it is usual to model this metastable state as the ground state of a system with a repulsive two body potential having the same scattering length as the true potential, and this is what we shall do. In this paper all potentials will be positive.

2. The Dilute Bose Gas in 3D

We consider the Hamiltonian for N bosons of mass m enclosed in a cubic box Λ of side length L and interacting by a spherically symmetric pair potential $v(|\vec{x}_i - \vec{x}_j|)$:

$$H_N = -\mu \sum_{i=1}^{N} \Delta_i + \sum_{1\leq i<j\leq N} v(|\vec{x}_i - \vec{x}_j|). \tag{2.1}$$

Here $\vec{x}_i \in \mathbb{R}^3$, $i = 1, \dots, N$ are the positions of the particles, Δ_i the Laplacian with respect to $\vec{x}_i$, and we have denoted $\hbar^2/2m$ by μ for short. (By choosing suitable units μ could, of course, be eliminated, but we want to keep track of the dependence of the energy on Planck's constant and the mass.) The Hamiltonian (2.1) operates on *symmetric* wave functions in

$L^2(\Lambda^N, d\vec{x}_1 \cdots d\vec{x}_N)$ as is appropriate for bosons. The interaction potential will be assumed to be *nonnegative* and to decrease faster than $1/r^3$ at infinity.

We are interested in the ground state energy $E_0(N, L)$ of (2.1) in the *thermodynamic limit* when N and L tend to infinity with the density $\rho = N/L^3$ fixed. The energy per particle in this limit is

$$e_0(\rho) = \lim_{L\to\infty} E_0(\rho L^3, L)/(\rho L^3). \tag{2.2}$$

Our results about $e_0(\rho)$ are based on estimates on $E_0(N, L)$ for finite N and L, which are important, e.g., for the considerations of inhomogeneous systems in [LSeY1]. To define $E_0(N, L)$ precisely one must specify the boundary conditions. These should not matter for the thermodynamic limit. To be on the safe side we use Neumann boundary conditions for the lower bound, and Dirichlet boundary conditions for the upper bound since these lead, respectively, to the lowest and the highest energies.

For experiments with dilute gases the *low density asymptotics* of $e_0(\rho)$ is of importance. Low density means here that the mean interparticle distance, $\rho^{-1/3}$ is much larger than the *scattering length* a of the potential, which is defined as follows. The zero energy scattering Schrödinger equation

$$-2\mu\Delta\psi + v(r)\psi = 0 \tag{2.3}$$

has a solution of the form, asymptotically as $|\vec{x}| = r \to \infty$ (or for all $r > R_0$ if $v(r) = 0$ for $r > R_0$),

$$\psi_0(\vec{x}) = 1 - a/|\vec{x}| \tag{2.4}$$

(The factor 2 in (2.3) comes from the reduced mass of the two particle problem.) Writing $\psi_0(\vec{x}) = u_0(|\vec{x}|)/|\vec{x}|$ this is the same as

$$a = \lim_{r\to\infty} r - \frac{u_0(r)}{u_0'(r)}, \tag{2.5}$$

where u_0 solves the zero energy (radial) scattering equation,

$$-2\mu u_0''(r) + v(r)u_0(r) = 0 \tag{2.6}$$

with $u_0(0) = 0$.

An important special case is the hard core potential $v(r) = \infty$ if $r < a$ and $v(r) = 0$ otherwise. Then the scattering length a and the radius a are the same.

Our main result is a rigorous proof of the formula

$$e_0(\rho) \approx 4\pi\mu\rho a \tag{2.7}$$

for $\rho a^3 \ll 1$, more precisely of

Theorem 2.1 (Low density limit of the ground state energy).

$$\lim_{\rho a^3\to 0} \frac{e_0(\rho)}{4\pi\mu\rho a} = 1. \tag{2.8}$$

This formula is independent of the boundary conditions used for the definition of $e_0(\rho)$. It holds for every positive radially symmetric pair potential such that $\int_R^\infty v(r)r^2 dr < \infty$ for some R, which guarantees a finite scattering length, cf. Appendix A in [LY2].

The genesis of an understanding of $e_0(\rho)$ was the pioneering work [Bo] of Bogolubov, and in the 50's and early 60's several derivations of (2.8) were presented [HY], [L1], even including higher order terms:

$$\frac{e_0(\rho)}{4\pi\mu\rho a} = 1 + \tfrac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8\left(\tfrac{4\pi}{3} - \sqrt{3}\right)(\rho a^3)\log(\rho a^3) + O(\rho a^3) \quad (2.9)$$

These early developments are reviewed in [L2]. They all rely on some special assumptions about the ground state that have never been proved, or on the selection of special terms from a perturbation series which likely diverges. The only rigorous estimates of this period were established by Dyson, who derived the following bounds in 1957 for a gas of hard spheres [D1]:

$$\frac{1}{10\sqrt{2}} \le \frac{e_0(\rho)}{4\pi\mu\rho a} \le \frac{1 + 2Y^{1/3}}{(1 - Y^{1/3})^2} \quad (2.10)$$

with $Y = 4\pi\rho a^3/3$. While the upper bound has the asymptotically correct form, the lower bound is off the mark by a factor of about 1/14. But for about 40 years this was the best lower bound available!

Under the assumption that (2.8) is a correct asymptotic formula for the energy, we see at once that understanding it physically, much less proving it, is not a simple matter. Initially, the problem presents us with two lengths, $a \ll \rho^{-1/3}$ at low density. However, (2.8) presents us with another length generated by the solution to the problem. This length is the de Broglie wavelength, or 'uncertainty principle' length (sometimes called 'healing length')

$$\ell_c \sim (\rho a)^{-1/2}. \quad (2.11)$$

The reason for saying that ℓ_c is the de Broglie wavelength is that in the hard core case all the energy is kinetic (the hard core just imposes a $\psi = 0$ boundary condition whenever the distance between two particles is less than a). By the uncertainty principle, the kinetic energy is proportional to an inverse length squared, namely ℓ_c. We then have the relation (since ρa^3 is small)

$$a \ll \rho^{-1/3} \ll \ell_c \quad (2.12)$$

which implies, physically, that it is impossible to localize the particles relative to each other (even though ρ is small). Bosons in their ground state are therefore 'smeared out' over distances large compared to the mean particle distance and their individuality is entirely lost. They cannot be localized with respect to each other without changing the kinetic energy enormously.

Fermions, on the other hand, prefer to sit in 'private rooms', i.e., ℓ_c is never bigger than $\rho^{-1/3}$ by a fixed factor. In this respect the quantum nature of bosons is much more pronounced than for fermions.

Since (2.8) is a basic result about the Bose gas it is clearly important to derive it rigorously and in reasonable generality, in particular for more general cases than hard spheres. The question immediately arises for which interaction potentials one may expect it to be true. A notable fact is that it *not true for all* v with $a > 0$, since there are two body potentials with positive scattering length that allow many body bound states. (There are even such potentials without two body bound states but with three body bound states [Ba].) For such potentials (2.8) is clearly false. Our proof, presented in the sequel, works for nonnegative v, but we conjecture that (2.8) holds if $a > 0$ and v has no N-body bound states for any N. The lower bound is, of course, the hardest part, but the upper bound is not altogether trivial either.

Before we start with the estimates a simple computation and some heuristics may be helpful to make (2.8) plausible and motivate the formal proofs.

With ψ_0 the zero energy scattering solution, partial integration, using (2.3) and (2.4), gives, for $R \geq R_0$,

$$\int_{|\vec{x}|\leq R} \{2\mu|\nabla\psi_0|^2 + v|\psi_0|^2\}d\vec{x} = 8\pi\mu a\left(1 - \frac{a}{R}\right) \to 8\pi\mu a \quad \text{for } R \to \infty. \tag{2.13}$$

Moreover, for positive interaction potentials the scattering solution minimizes the quadratic form in (2.13) for each $R \geq R_0$ with the boundary condition $\psi_0(|\vec{x}| = R) = (1 - a/R)$. Hence the energy $E_0(2, L)$ of two particles in a large box, i.e., $L \gg a$, is approximately $8\pi\mu a/L^3$. If the gas is sufficiently dilute it is not unreasonable to expect that the energy is essentially a sum of all such two particle contributions. Since there are $N(N-1)/2$ pairs, we are thus lead to $E_0(N, L) \approx 4\pi\mu a N(N-1)/L^3$, which gives (2.8) in the thermodynamic limit.

This simple heuristics is far from a rigorous proof, however, especially for the lower bound. In fact, it is rather remarkable that the same asymptotic formula holds both for 'soft' interaction potentials, where perturbation theory can be expected to be a good approximation, and potentials like hard spheres where this is not so. In the former case the ground state is approximately the constant function and the energy is *mostly potential*: According to perturbation theory $E_0(N, L) \approx N(N-1)/(2L^3)\int v(|\vec{x}|)d\vec{x}$. In particular it is *independent of* μ, i.e. of Planck's constant and mass. Since, however, $\int v(|\vec{x}|)d\vec{x}$ is the first Born approximation to $8\pi\mu a$ (note that a depends on μ!), this is not in conflict with (2.8). For 'hard' potentials on the other hand, the ground state is *highly correlated*, i.e., it is far from being a product of single particle states. The energy is here *mostly kinetic*, because the wave function is very small where the potential is large. These two quite different regimes, the potential energy dominated one and the kinetic energy dominated one, cannot be distinguished by the low density asymptotics of the energy. Whether they behave differently with respect to other phenomena, e.g., Bose-Einstein condensation, is not known at present.

Bogolubov's analysis [Bo] presupposes the existence of Bose-Einstein condensation. Nevertheless, it is correct (for the energy) for the one-dimensional delta-function Bose gas [LL], despite the fact that there is (presumably) no condensation in that case [PiSt]. It turns out that BE condensation is not really needed in order to understand the energy. As we shall see, 'global' condensation can be replaced by a 'local' condensation on boxes whose size is independent of L. It is this crucial understanding that enables us to prove Theorem 1.1 without having to decide about BE condensation.

An important idea of Dyson was to transform the hard sphere potential into a soft potential at the cost of sacrificing the kinetic energy, i.e., effectively to move from one regime to the other. We shall make use of this idea in our proof of the lower bound below. But first we discuss the simpler upper bound, which relies on other ideas from Dyson's beautiful paper [D1].

2.1. **Upper Bound.** The following generalization of Dyson's upper bound holds [LSeY1], [Se1]:

Theorem 2.2 (**Upper bound**). *Define* $\rho_1 = (N-1)/L^3$ *and* $b = (4\pi\rho_1/3)^{-1/3}$. *For nonnegative potentials* v *and* $b > a$ *the ground state energy of (2.1) with periodic boundary conditions satisfies*

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \frac{a}{b} + \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1-\frac{a}{b}\right)^8}. \tag{2.14}$$

For Dirichlet boundary conditions the estimate holds with (const.)$/L^2$ *added to the right side. Thus in the thermodynamic limit and for all boundary conditions*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \leq \frac{1 - Y^{1/3} + Y^{2/3} - \frac{1}{2}Y}{(1-Y^{1/3})^8}. \tag{2.15}$$

provided $Y = 4\pi\rho a^3/3 < 1$.

Remark. The bound (2.14) holds for potentials with infinite range, provided $b > a$. For potentials of finite range R_0 it can be improved for $b > R_0$ to

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1-\frac{a}{b}\right)^4}. \tag{2.16}$$

Proof. We first remark that the expectation value of (2.1) with any trial wave function gives an upper bound to the bosonic ground state energy, even if the trial function is not symmetric under permutations of the variables. The reason is that an absolute ground state of the elliptic differential operator (2.1) (i.e., a ground state without symmetry requirement) is a nonnegative function which can be be symmetrized without changing the energy because (2.1) is symmetric under permutations. In other words, the absolute ground state energy is the same as the bosonic ground state energy.

Following [D1] we choose a trial function of the following form

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) = F_1(\vec{x}_1) \cdot F_2(\vec{x}_1, \vec{x}_2) \cdots F_N(\vec{x}_1, \ldots, \vec{x}_N). \tag{2.17}$$

More specifically, $F_1 \equiv 1$ and F_i depends only on the distance of $\vec{x}_i$ to its nearest neighbor among the the points $\vec{x}_1, \ldots, \vec{x}_{i-1}$ (taking the periodic boundary into account):

$$F_i(\vec{x}_1, \ldots, \vec{x}_i) = f(t_i), \quad t_i = \min\left(|\vec{x}_i - \vec{x}_j|, j = 1, \ldots, i-1\right), \tag{2.18}$$

with a function f satisfying

$$0 \leq f \leq 1, \quad f' \geq 0. \tag{2.19}$$

The intuition behind the ansatz (2.17) is that the particles are inserted into the system one at the time, taking into account the particles previously inserted. While such a wave function cannot reproduce all correlations present in the true ground state, it turns out to capture the leading term in the energy for dilute gases. The form (2.17) is computationally easier to handle than an ansatz of the type $\prod_{i<j} f(|\vec{x}_i - \vec{x}_j|)$, which might appear more natural in view of the heuristic remarks after Eq. (2.13).

The function f is chosen to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \leq r \leq b, \\ 1 & \text{for } r > b, \end{cases} \tag{2.20}$$

with $f_0(r) = u_0(r)/r$ the zero energy scattering solution defined by (2.6). The estimates (2.14) and (2.16) are obtained by somewhat lengthy computations similar as in [D1], but making use of (2.13). For details we refer to [LSeY1] and [Se1].

A test wave function with Dirichlet boundary condition may be obtained by localizing the wave function (2.17) on the length scale L. The energy cost per particle for this is (const.)$/L^2$. ■

2.2. **Lower Bound.** It was explained previously in this section why the lower bound for the bosonic ground state energy of (2.1) is not easy to obtain. The three different length scales (2.12) for bosons will play a role in the proof below.

- The scattering length a.
- The mean particle distance $\rho^{-1/3}$.
- The 'uncertainty principle length' ℓ_c, defined by $\mu\ell_c^{-2} = e_0(\rho)$, i.e., $\ell_c \sim (\rho a)^{-1/2}$.

Our lower bound for $e_0(\rho)$ is as follows.

Theorem 2.3 (**Lower bound in the thermodynamic limit**). *For a positive potential v with finite range and Y small enough*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \geq (1 - CY^{1/17}) \tag{2.21}$$

with C a constant. If v does not have finite range, but decreases faster than $1/r^3$ (more precisely, $\int_R^\infty v(r)r^2 dr < \infty$ for some R) then an analogous bound to (2.21) holds, but with $CY^{-1/17}$ replaced by $o(1)$ as $Y \to 0$.

It should be noted right away that the error term $-CY^{1/17}$ in (2.21) is of no fundamental significance and is not believed to reflect the true state of affairs. Presumably, it does not even have the right sign. We mention in passing that C can be taken to be 8.9 [Se1].

As mentioned at the beginning of this section after Eq. (2.2), a lower bound on $E_0(N, L)$ for finite N and L is of importance for applications to inhomogeneous gases, and in fact we derive (2.21) from such a bound. We state it in the following way:

Theorem 2.4 (**Lower bound in a finite box**). *For a positive potential v with finite range there is a $\delta > 0$ such that the ground state energy of (2.1) with Neumann boundary conditions satisfies*

$$E_0(N,L)/N \geq 4\pi\mu\rho a\left(1 - CY^{1/17}\right) \tag{2.22}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are positive constants, independent of N and L. (Note that the condition on L/a requires in particular that N must be large enough, $N >$ (const.)$Y^{-1/17}$.) As in Theorem 2.3 such a bound, but possibly with a different error term holds also for potentials v of infinite range that decrease sufficiently fast at infinity.

The first step in the proof of Theorem 2.4 is a generalization of a lemma of Dyson, which allows us to replace v by a 'soft' potential, at the cost of sacrificing kinetic energy and increasing the effective range.

Lemma 2.5. *Let $v(r) \geq 0$ with finite range R_0. Let $U(r) \geq 0$ be any function satisfying $\int U(r)r^2dr \leq 1$ and $U(r) = 0$ for $r < R_0$. Let $\mathcal{B} \subset \mathbb{R}^3$ be star shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then for all differentiable functions ψ*

$$\int_{\mathcal{B}} \left[\mu|\nabla\psi|^2 + \tfrac{1}{2}v|\psi|^2\right] \geq \mu a \int_{\mathcal{B}} U|\psi|^2. \tag{2.23}$$

Proof. Actually, (2.23) holds with $\mu|\nabla\psi(\vec{x})|^2$ replaced by the (smaller) radial kinetic energy, $\mu|\partial\psi(\vec{x})/\partial r|^2$, and it suffices to prove the analog of (2.23) for the integral along each radial line with fixed angular variables. Along such a line we write $\psi(\vec{x}) = u(r)/r$ with $u(0) = 0$. We consider first the special case when when U is a delta-function at some radius $R \geq R_0$, i.e.,

$$U(r) = \frac{1}{R^2}\delta(r - R). \tag{2.24}$$

For such U the analog of (2.23) along the radial line is

$$\int_0^{R_1} \{\mu[u'(r) - (u(r)/r)]^2 + \tfrac{1}{2}v(r)|u(r)|^2\}dr \geq \begin{cases} 0 & \text{if } R_1 < R \\ \mu a|u(R)|^2/R^2 & \text{if } R \leq R_1 \end{cases} \tag{2.25}$$

where R_1 is the length of the radial line segment in $\mathcal{B}$. The case $R_1 < R$ is trivial, because $\mu|\partial\psi/\partial r|^2 + \frac{1}{2}v|\psi|^2 \geq 0$. (Note that positivity of v is used here.) If $R \leq R_1$ we consider the integral on the the left side of (2.25) from 0 to R instead of R_1 and minimize it under the boundary condition that $u(0) = 0$ and $u(R)$ is a fixed constant. Since everything is homogeneous in u we may normalize this value to $u(R) = R - a$. This minimization problem leads to the zero energy scattering equation (2.6). Since v is positive, the solution is a true minimum and not just a stationary point.

Because $v(r) = 0$ for $r > R_0$ the solution, u_0, satisfies $u_0(r) = r - a$ for $r > R_0$. By partial integration,

$$\int_0^R \{\mu[u_0'(r) - (u_0(r)/r)]^2 + \tfrac{1}{2}v(r)|u_0(r)|^2\}dr = \mu a|R-a|/R \geq \mu a|R-a|^2/R^2. \tag{2.26}$$

But $|R-a|^2/R^2$ is precisely the right side of (2.25) if u satisfies the normalization condition.

This derivation of (2.23) for the special case (2.24) implies the general case, because every U can be written as a superposition of δ-functions, $U(r) = \int R^{-2}\delta(r-R)\,U(R)R^2dR$, and $\int U(R)R^2dR \leq 1$ by assumption. ■

By dividing Λ for given points $\vec{x}_1, \ldots, \vec{x}_N$ into Voronoi cells $\mathcal{B}_i$ that contain all points closer to $\vec{x}_i$ than to $\vec{x}_j$ with $j \neq i$ (these cells are star shaped w.r.t. $\vec{x}_i$, indeed convex), the following corollary of Lemma 2.5 can be derived in the same way as the corresponding Eq. (28) in [D1].

Corollary 2.6. *For any U as in Lemma 2.5*

$$H_N \geq \mu a W \tag{2.27}$$

with

$$W(\vec{x}_1, \ldots, \vec{x}_N) = \sum_{i=1}^N U(t_i), \tag{2.28}$$

where t_i is the distance of $\vec{x}_i$ to its nearest neighbor among the other points $\vec{x}_j$, $j = 1, \ldots, N$, i.e.,

$$t_i(\vec{x}_1, \ldots, \vec{x}_N) = \min_{j,\, j\neq i} |\vec{x}_i - \vec{x}_j|. \tag{2.29}$$

(Note that t_i has here a slightly different meaning than in (2.18), where it denoted the distance to the nearest neighbor among the $\vec{x}_j$ with $j \leq i-1$.)

Dyson considers in [D1] a one parameter family of U's that is essentially the same as the following choice, which is convenient for the present purpose:

$$U_R(r) = \begin{cases} 3(R^3 - R_0^3)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise.} \end{cases} \tag{2.30}$$

We denote the corresponding interaction (2.28) by W_R. For the hard core gas one obtains

$$E(N,L) \geq \sup_R \inf_{(\vec{x}_1,\ldots,\vec{x}_N)} \mu a W_R(\vec{x}_1, \ldots, \vec{x}_N) \tag{2.31}$$

where the infimum is over $(\vec{x}_1, \ldots, x_N) \in \Lambda^N$ with $|\vec{x}_i - \vec{x}_j| \geq R_0 = a$, because of the hard core. At fixed R simple geometry gives

$$\inf_{(\vec{x}_1,\ldots,\vec{x}_N)} W_R(\vec{x}_1, \ldots, \vec{x}_N) \geq \left(\frac{A}{R^3} - \frac{B}{\rho R^6} \right) \tag{2.32}$$

with certain constants A and B. An evaluation of these constants gives Dyson's bound

$$E(N,L)/N \geq \frac{1}{10\sqrt{2}} 4\pi\mu\rho a. \tag{2.33}$$

The main reason this method does not give a better bound is that R must be chosen quite big, namely of the order of the mean particle distance $\rho^{-1/3}$, in order to guarantee that the spheres of radius R around the N points overlap. Otherwise the infimum of W_R will be zero. But large R means that W_R is small. It should also be noted that this method does not work for potentials other than hard spheres: If $|\vec{x}_i - \vec{x}_j|$ is allowed to be less than R_0, then the right side of (2.31) is zero because $U(r) = 0$ for $r < R_0$.

For these reasons we take another route. We still use Lemma 2.5 to get into the soft potential regime, but we do *not* sacrifice *all* the kinetic energy as in (2.27). Instead we write, for $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1-\varepsilon)H_N \geq \varepsilon T_N + (1-\varepsilon)H_N \tag{2.34}$$

with $T_N = -\sum_i \Delta_i$ and use (2.27) only for the part $(1-\varepsilon)H_N$. This gives

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu a W_R. \tag{2.35}$$

We consider the operator on the right side from the viewpoint of first order perturbation theory, with εT_N as the unperturbed part, denoted H_0.

The ground state of H_0 in a box of side length L is $\Psi_0(\vec{x}_1, \ldots, \vec{x}_N) \equiv L^{-3N/2}$ and we denote expectation values in this state by $\langle \cdot \rangle_0$. A computation, cf. Eq. (21) in [LY1], gives

$$\begin{aligned} 4\pi\rho\left(1 - \tfrac{1}{N}\right) &\geq \langle W_R \rangle_0 / N \\ &\geq 4\pi\rho\left(1 - \tfrac{1}{N}\right)\left(1 - \tfrac{2R}{L}\right)^3 \left(1 + 4\pi\rho(1 - \tfrac{1}{N})(R^3 - R_0^3)/3)\right)^{-1}. \end{aligned} \tag{2.36}$$

The rationale behind the various factors is as follows: $(1 - \frac{1}{N})$ comes from the fact that the number of pairs is $N(N-1)/2$ and not $N^2/2$, $(1-2R/L)^3$ takes into account the fact that the particles do not interact beyond the boundary of Λ, and the last factor measures the probability to find another particle within the interaction range of the potential U_R for a given particle.

The estimates (2.36) on the first order term look at first sight quite promising, for if we let $L \to \infty$, $N \to \infty$ with $\rho = N/L^3$ fixed, and subsequently take $R \to \infty$, then $\langle W_R \rangle_0 / N$ converges to $4\pi\rho$, which is just what is desired. But the first order result (2.36) is not a rigorous bound on $E_0(N,L)$, we need *error estimates*, and these will depend on ε, R and L.

We now recall *Temple's inequality* [T] for the expectation values of an operator $H = H_0 + V$ in the ground state $\langle\cdot\rangle_0$ of H_0. It is a simple consequence of the operator inequality

$$(H - E_0)(H - E_1) \geq 0 \tag{2.37}$$

for the two lowest eigenvalues, $E_0 < E_1$, of H and reads

$$E_0 \geq \langle H\rangle_0 - \frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0} \tag{2.38}$$

provided $E_1 - \langle H\rangle_0 > 0$. Furthermore, if $V \geq 0$ we may use $E_1 \geq E_1^{(0)}=$ second lowest eigenvalue of H_0 and replace E_1 in (2.38) by $E_1^{(0)}$.

From (2.36) and (2.38) we get the estimate

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1 - \mathcal{E}(\rho, L, R, \varepsilon)) \tag{2.39}$$

with

$$\begin{aligned} 1 - \mathcal{E}(\rho, L, R, \varepsilon) \;&=\; (1-\varepsilon)\left(1 - \tfrac{1}{\rho L^3}\right)\left(1 - \tfrac{2R}{L}\right)^3 \left(1 + \tfrac{4\pi}{3}\rho(1 - \tfrac{1}{N})(R^3 - R_0^3)\right)^{-1} \\ &\times \left(1 - \frac{\mu a\big(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2\big)}{\langle W_R\rangle_0\big(E_1^{(0)} - \mu a\langle W_R\rangle_0\big)}\right). \end{aligned} \tag{2.40}$$

To evaluate this further one may use the estimates (2.36) and the bound

$$\langle W_R^2\rangle_0 \leq 3\frac{N}{R^3 - R_0^3}\langle W_R\rangle_0 \tag{2.41}$$

which follows from $U_R^2 = 3(R^3 - R_0^3)^{-1}U_R$ together with the Cauchy-Schwarz inequality. A glance at the form of the error term reveals, however, that it is *not* possible here to take the thermodynamic limit $L \to \infty$ with ρ fixed: We have $E_1^{(0)} = \varepsilon\pi\mu/L^2$ (this is the kinetic energy of a *single* particle in the first excited state in the box), and the factor $E_1^{(0)} - \mu a\langle W_R\rangle_0$ in the denominator in (2.40) is, up to unimportant constants and lower order terms, $\sim (\varepsilon L^{-2} - a\rho^2 L^3)$. Hence the denominator eventually becomes negative and Temple's inequality looses its validity if L is large enough.

As a way out of this dilemma we divide the big box Λ into cubic *cells* of side length ℓ that is kept *fixed* as $L \to \infty$. The number of cells, L^3/ℓ^3, on the other hand, increases with L. The N particles are distributed among these cells, and we use (2.40), with L replaced by ℓ, N by the particle number, n, in a cell and ρ by n/ℓ^3, to estimate the energy in each cell with *Neumann* conditions on the boundary. For each distribution of the particles we add the contributions from the cells, neglecting interactions across boundaries. Since $v \geq 0$ by assumption, this can only lower the energy. Finally, we minimize over all possible choices of the particle numbers for the various cells adding up to N. The energy obtained in this way is a lower bound to $E_0(N,L)$, because we are effectively allowing discontinuous test functions for the quadratic form given by H_N.

In mathematical terms, the cell method leads to

$$E_0(N,L)/N \geq (\rho\ell^3)^{-1} \inf \sum_{n\geq 0} c_n E_0(n,\ell) \tag{2.42}$$

where the infimum is over all choices of coefficients $c_n \geq 0$ (relative number of cells containing exactly n particles), satisfying the constraints

$$\sum_{n\geq 0} c_n = 1, \qquad \sum_{n\geq 0} c_n n = \rho\ell^3. \tag{2.43}$$

The minimization problem for the distributions of the particles among the cells would be easy if we knew that the ground state energy $E_0(n,\ell)$ (or a good lower bound to it) were convex in n. Then we could immediately conclude that it is best to have the particles as evenly distributed among the boxes as possible, i.e., c_n would be zero except for the n equal to the integer closest to $\rho\ell^3$. This would give

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1-\mathcal{E}(\rho,\ell,R,\varepsilon)) \tag{2.44}$$

i.e., replacement of L in (2.39) by ℓ, which is independent of L. The blow up of $\mathcal{E}$ for $L\to\infty$ would thus be avoided.

Since convexity of $E_0(n,\ell)$ is not known (except in the thermodynamic limit) we must resort to other means to show that $n = O(\rho\ell^3)$ in all boxes. The rescue comes from *superadditivity* of $E_0(n,\ell)$, i.e., the property

$$E_0(n+n',\ell) \geq E_0(n,\ell) + E_0(n',\ell) \tag{2.45}$$

which follows immediately from $v \geq 0$ by dropping the interactions between the n particles and the n' particles. The bound (2.45) implies in particular that for any $n,p \in \mathbb{N}$ with $n \geq p$

$$E(n,\ell) \geq [n/p]\,E(p,\ell) \geq \frac{n}{2p}E(p,\ell) \tag{2.46}$$

since the largest integer $[n/p]$ smaller than n/p is in any case $\geq n/(2p)$.

The way (2.46) is used is as follows: Replacing L by ℓ, N by n and ρ by n/ℓ^3 in (2.39) we have for fixed R and ε

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1)K(n,\ell) \tag{2.47}$$

with a certain function $K(n,\ell)$ determined by (2.40). We shall see that K is monotonously decreasing in n, so that if $p\in\mathbb{N}$ and $n\leq p$ then

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1)K(p,\ell). \tag{2.48}$$

We now split the sum in (2.42) into two parts. For $n<p$ we use (2.48), and for $n\geq p$ we use (2.46) together with (2.48) for $n=p$. The task is thus to minimize

$$\sum_{n<p} c_n n(n-1) + \tfrac{1}{2}\sum_{n\geq p} c_n n(p-1) \tag{2.49}$$

subject to the constraints (2.43). Putting

$$k := \rho\ell^3 \quad \text{and} \quad t := \sum_{n<p} c_n n \le k \tag{2.50}$$

we have $\sum_{n\ge p} c_n n = k - t$, and since $n(n-1)$ is convex in n and vanishes for $n = 0$, and $\sum_{n<p} c_n \le 1$, the expression (2.49) is

$$\ge t(t-1) + \tfrac{1}{2}(k-t)(p-1). \tag{2.51}$$

We have to minimize this for $1 \le t \le k$. If $p \ge 4k$ the minimum is taken at $t = k$ and is equal to $k(k-1)$. Altogether we have thus shown that

$$\frac{E_0(N,L)}{N} \ge 4\pi\mu a\rho \left(1 - \frac{1}{\rho\ell^3}\right) K(4\rho\ell^3, \ell). \tag{2.52}$$

What remains is to take a closer look at $K(4\rho\ell^3, \ell)$, which depends on the parameters ε and R besides ℓ, and choose the parameters in an optimal way. From (2.40) and (2.41) we obtain

$$\begin{aligned} K(n,\ell) &= (1-\varepsilon)\left(1 - \tfrac{2R}{\ell}\right)^3 \left(1 + \tfrac{4\pi}{3}\rho(1 - \tfrac{1}{n})(R^3 - R_0^3)\right)^{-1} \\ &\times \left(1 - \frac{3}{\pi}\frac{an}{(R^3 - R_0^3)(\varepsilon\ell^{-2} - 4a\ell^{-3}n(n-1))}\right). \end{aligned} \tag{2.53}$$

The estimate (2.47) with this K is valid as long as the denominator in the last factor in (2.53) is ≥ 0, and in order to have a formula for all n we can take 0 as a trivial lower bound in other cases or when (2.47) is negative. As required for (2.48), K is monotonously decreasing in n. We now insert $n = 4\rho\ell^3$ and obtain

$$\begin{aligned} K(4\rho\ell^3,\ell) &\ge (1-\varepsilon)\left(1 - \tfrac{2R}{\ell}\right)^3 \left(1 + (\text{const.})Y(\ell/a)^3(R^3 - R_0^3)/\ell^3\right)^{-1} \\ &\times \left(1 - \frac{\ell^3}{(R^3 - R_0^3)}\frac{(\text{const.})Y}{(\varepsilon(a/\ell)^2 - (\text{const.})Y^2(\ell/a)^3)}\right) \end{aligned} \tag{2.54}$$

with $Y = 4\pi\rho a^3/3$ as before. Also, the factor

$$\left(1 - \frac{1}{\rho\ell^3}\right) = (1 - (\text{const.})Y^{-1}(a/\ell)^3) \tag{2.55}$$

in (2.52) (which is the ratio between $n(n-1)$ and n^2) must not be be forgotten. We now make the ansatz

$$\varepsilon \sim Y^\alpha, \quad a/\ell \sim Y^\beta, \quad (R^3 - R_0^3)/\ell^3 \sim Y^\gamma \tag{2.56}$$

with exponents α, β and γ that we choose in an optimal way. The conditions to be met are as follows:

- $\varepsilon(a/\ell)^2 - (\text{const.})Y^2(\ell/a)^3 > 0$. This holds for all small enough Y, provided $\alpha + 5\beta < 2$ which follows from the conditions below.
- $\alpha > 0$ in order that $\varepsilon \to 0$ for $Y \to 0$.
- $3\beta - 1 > 0$ in order that $Y^{-1}(a/\ell)^3 \to 0$ for for $Y \to 0$.
- $1 - 3\beta + \gamma > 0$ in order that $Y(\ell/a)^3(R^3 - R_0^3)/\ell^3 \to 0$ for for $Y \to 0$.
- $1 - \alpha - 2\beta - \gamma > 0$ to control the last factor in (2.54).

Taking

$$\alpha = 1/17, \quad \beta = 6/17, \quad \gamma = 3/17 \tag{2.57}$$

all these conditions are satisfied, and

$$\alpha = 3\beta - 1 = 1 - 3\beta + \gamma = 1 - \alpha - 2\beta - \gamma = 1/17. \tag{2.58}$$

It is also clear that $2R/\ell \sim Y^{\gamma/3} = Y^{1/17}$, up to higher order terms. This completes the proof of Theorems 2.3 and 2.4, for the case of potentials with finite range. By optimizing the proportionality constants in (2.56) one can show that $C = 8.9$ is possible in Theorem 2.3 [Se1]. The extension to potentials of infinite range but finite scattering length is obtained by approximation by finite range potentials, controlling the change of the scattering length as the cut-off is removed. See Appendix A in [LY2] and Appendix B in [LSeY1] for details. We remark that a slower decrease of the potential than $1/r^3$ implies infinite scattering length. ■

The exponents (2.57) mean in particular that

$$a \ll R \ll \rho^{-1/3} \ll \ell \ll (\rho a)^{-1/2}, \tag{2.59}$$

whereas Dyson's method required $R \sim \rho^{-1/3}$ as already explained. The condition $\rho^{-1/3} \ll \ell$ is required in order to have many particles in each box and thus $n(n-1) \approx n^2$. The condition $\ell \ll (\rho a)^{-1/2}$ is necessary for a spectral gap gap $\gg e_0(\rho)$ in Temple's inequality. It is also clear that this choice of ℓ would lead to a far too big energy and no bound for $e_0(\rho)$ if we had chosen Dirichlet instead of Neumann boundary conditions for the cells. But with the latter the method works!

3. The Dilute Bose Gas in 2D

In contrast to the three-dimensional theory, the two-dimensional Bose gas began to receive attention only relatively late. The first derivation of the correct asymptotic formula was, to our knowledge, done by Schick [S] for a gas of hard discs. He found

$$e(\rho) \approx 4\pi\mu\rho|\ln(\rho a^2)|^{-1}. \tag{3.1}$$

This was accomplished by an infinite summation of 'perturbation series' diagrams. Subsequently, a corrected modification of [S] was given in [HFM]. Positive temperature extensions were given in [Po] and in [FH]. All this work involved an analysis in momentum space, with the exception of a method due to one of us that works directly in configuration space [L1]. Ovchinnikov [O] derived (3.1) by using, basically, the method in [L1]. These derivations require several unproven assumptions and are not rigorous.

In two dimensions the scattering length a is defined using the zero energy scattering equation (2.3) but instead of $\psi(r) \approx 1 - a/r$ we now impose the asymptotic condition $\psi(r) \approx \ln(r/a)$. This is explained in the appendix to [LY2].

Note that in two dimensions the ground state energy could not possibly be $e_0(\rho) \approx 4\pi\mu\rho a$ as in three dimensions because that would be dimensionally wrong. Since $e_0(\rho)$ should essentially be proportional to ρ, there is apparently no room for an a dependence — which is ridiculous! It turns out that this dependence comes about in the $\ln(\rho a^2)$ factor.

One of the intriguing facts about (3.1) is that the energy for N particles is *not equal* to $N(N-1)/2$ times the energy for two particles in the low density limit — as is the case in three dimensions. The latter quantity, $E_0(2,L)$, is, asymptotically for large L, equal to $8\pi\mu L^{-2}\left[\ln(L^2/a^2)\right]^{-1}$. (This is seen in an analogous way as (2.13). The three-dimensional boundary condition $\psi_0(|\vec{x}|=R) = 1 - a/R$ is replaced by $\psi_0(|\vec{x}|=R) = \ln(R/a)$ and moreover it has to be taken into account that with this normalization $\|\psi_0\|^2 = (\text{volume})(\ln(R/a))^2$ (to leading order), instead of just the volume in the three-dimensional case.) Thus, if the $N(N-1)/2$ rule were to apply, (3.1) would have to be replaced by the much smaller quantity $4\pi\mu\rho\left[\ln(L^2/a^2)\right]^{-1}$. In other words, L, which tends to ∞ in the thermodynamic limit, has to be replaced by the mean particle separation, $\rho^{-1/2}$ in the logarithmic factor. Various poetic formulations of this curious fact have been given, but the fact remains that the non-linearity is something that does not occur in more than two dimensions and its precise nature is hardly obvious, physically. This anomaly is the main reason that the two-dimensional case is not a trivial extension of the three-dimensional one.

Eq. (3.1) was proved in [LY2] for nonnegative, finite range two-body potentials by finding upper and lower bounds of the correct form, using similar ideas as in the previous section for the three-dimensional case. We discuss below the modifications that have to be made in the present two-dimensional case. The restriction to finite range can be relaxed as in three dimensions, but the restriction to nonnegative v cannot be removed in the current state of our methodology. The upper bounds will have relative remainder terms $\mathrm{O}(|\ln(\rho a^2)|^{-1})$ while the lower bound will have remainder $\mathrm{O}(|\ln(\rho a^2)|^{-1/5})$. It is claimed in [HFM] that the relative error for a hard core gas is negative and $\mathrm{O}(\ln|\ln(\rho a^2)||\ln(\rho a^2)|^{-1})$, which is consistent with our bounds.

The upper bound is derived in complete analogy with the three dimensional case. The function f_0 in the variational ansatz (2.20) is in two dimensions also the zero energy scattering solution — but for 2D, of course. The result is

$$E_0(N,L)/N \leq \frac{2\pi\mu\rho}{\ln(b/a) - \pi\rho b^2}\left(1 + \mathrm{O}([\ln(b/a)]^{-1})\right). \tag{3.2}$$

The minimum over b of the leading term is obtained for $b = (2\pi\rho)^{-1/2}$. Inserting this in (3.2) we thus obtain

$$E_0(N,L)/N \leq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}\left(1 + \mathrm{O}(|\ln(\rho a^2)|^{-1}\right). \tag{3.3}$$

To prove the lower bound the essential new step is to modify Dyson's lemma for 2D. The 2D version of Lemma 2.5 is:

Lemma 3.1. *Let $v(r) \geq 0$ and $v(r) = 0$ for $r > R_0$. Let $U(r) \geq 0$ be any function satisfying*

$$\int_0^\infty U(r)\ln(r/a) r dr \leq 1 \text{ and } U(r) = 0 \text{ for } r < R_0. \tag{3.4}$$

Let $\mathcal{B} \subset \mathbb{R}^2$ be star-shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then, for all functions ψ in the Sobolev space $H^1(\mathcal{B})$,

$$\int_{\mathcal{B}} \left(\mu|\nabla\psi(\vec{x})|^2 + \tfrac{1}{2}v(|\vec{x}|)|\psi(\vec{x})|^2\right)\, d\vec{x} \geq \mu \int_{\mathcal{B}} U(|\vec{x}|)|\psi(\vec{x})|^2\, d\vec{x}. \tag{3.5}$$

Proof. In polar coordinates, r, θ, one has $|\nabla\psi|^2 \geq |\partial\psi/\partial r|^2$. Therefore, it suffices to prove that for each angle $\theta \in [0, 2\pi)$, and with $\psi(r,\theta)$ denoted simply by $f(r)$,

$$\int_0^{R(\theta)} \left(\mu|\partial f(r)/\partial r|^2 + \tfrac{1}{2}v(r)|f(r)|^2\right) r dr \geq \mu \int_0^{R(\theta)} U(r)|f(r)|^2\, r dr, \tag{3.6}$$

where $R(\theta)$ denotes the distance of the origin to the boundary of $\mathcal{B}$ along the ray θ.

If $R(\theta) \leq R_0$ then (3.6) is trivial because the right side is zero while the left side is evidently nonnegative. (Here, $v \geq 0$ is used.)

If $R(\theta) > R_0$ for some given value of θ, consider the disc $\mathcal{D}(\theta) = \{\vec{x} \in \mathbb{R}^2 \;:\; 0 \leq |\vec{x}| \leq R(\theta)\}$ centered at the origin in $\mathbb{R}^2$ and of radius $R(\theta)$. Our function f defines a spherically symmetric function, $\vec{x} \mapsto f(|\vec{x}|)$ on $\mathcal{D}(\theta)$, and (3.6) is equivalent to

$$\int_{\mathcal{D}(\theta)} \left(\mu|\nabla f(|\vec{x}|)|^2 + \frac{1}{2}v(|\vec{x}|)|f(|\vec{x}|)|^2\right) d\vec{x} \geq \mu \int_{\mathcal{D}(\theta)} U(|\vec{x}|)|f(|\vec{x}|)|^2 d\vec{x}. \tag{3.7}$$

Now choose some $R \in (R_0,\ R(\theta))$ and note that the left side of (3.7) is not smaller than the same quantity with $\mathcal{D}(\theta)$ replaced by the smaller disc $\mathcal{D}_R = \{\vec{x} \in \mathbb{R}^2 \;:\; 0 \leq |\vec{x}| \leq R\}$. (Again, $v \geq 0$ is used.) We now minimize this integral over $\mathcal{D}_R$, fixing $f(R)$. This minimization problem leads to the zero energy scattering equation. Plugging in the solution and integrating by parts leads to

$$2\pi \int_0^{R(\theta)} \left(\mu|\partial f(r)/\partial r|^2 + \frac{1}{2}v(r)|f(r)|^2\right) r dr \geq \frac{2\pi\mu}{\ln(R/a)}|f(R)|^2. \tag{3.8}$$

The proof is completed by multiplying both sides of (3.8) by $U(R)R\ln(R/a)$ and integrating with respect to R from R_0 to $R(\theta)$. ∎

As in Corollary 2.6, Lemma 3.1 can be used to bound the many body Hamiltonian H_N from below, as follows:

Corollary 3.2. *For any U as in Lemma 3.1 and any $0 < \varepsilon < 1$*

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu W \tag{3.9}$$

with $T_N = -\mu\sum_{i=1}^N \Delta_i$ *and*

$$W(\vec{x}_1,\dots,\vec{x}_N) = \sum_{i=1}^N U\left(\min_{j, j\neq i}|\vec{x}_i - \vec{x}_j|.\right). \tag{3.10}$$

For U we choose the following functions, parameterized by $R > R_0$:

$$U_R(r) = \begin{cases} \nu(R)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise} \end{cases} \tag{3.11}$$

with $\nu(R)$ chosen so that

$$\int_{R_0}^R U_R(r)\ln(r/a) r\, dr = 1 \tag{3.12}$$

for all $R > R_0$, i.e.,

$$\nu(R) = \int_{R_0}^R \ln(r/a) r\, dr = \tfrac{1}{4}\left\{R^2\left(\ln(R^2/a^2) - 1\right) - R_0^2\left(\ln(R_0^2/a^2) - 1\right)\right\}. \tag{3.13}$$

The nearest neighbor interaction (3.10) corresponding to U_R will be denoted W_R.

As in Subsection 2.2 we shall need estimates on the expectation value, $\langle W_R\rangle_0$, of W_R in the ground state of εT_N of (3.9) with Neumann boundary conditions. This is just the average value of W_R in a hypercube in $\mathbb{R}^{2N}$. Besides the normalization factor $\nu(R)$, the computation involves the volume (area) of the support of U_R, which is

$$A(R) = \pi(R^2 - R_0^2). \tag{3.14}$$

In contrast to the three-dimensional situation the normalization factor $\nu(R)$ is not just a constant (R independent) multiple of $A(R)$; the factor $\ln(r/a)$ in (3.4) accounts for the more complicated expressions in the two-dimensional case. Taking into account that U_R is proportional to the characteristic function of a disc of radius R with a hole of radius R_0, the following inequalities for n particles in a box of side length ℓ are obtained by the same geometric reasoning as lead to (2.36), cf. [LY1]:

$$\langle W_R\rangle_0 \geq \frac{n}{\nu(R)}\left(1 - \tfrac{2R}{\ell}\right)^2\left[1 - (1-Q)^{(n-1)}\right] \tag{3.15}$$

$$\langle W_R\rangle_0 \leq \frac{n}{\nu(R)}\left[1 - (1-Q)^{(n-1)}\right] \tag{3.16}$$

with

$$Q = A(R)/\ell^2 \tag{3.17}$$

being the relative volume occupied by the support of the potential U_R. Since $U_R^2 = \nu(R)^{-1}U_R$ we also have

$$\langle W_R^2\rangle_0 \leq \frac{n}{\nu(R)}\langle W_R\rangle_0. \tag{3.18}$$

As in [LY1] we estimate $[1-(1-Q)^{(n-1)}]$ by

$$(n-1)Q \geq \left[1-(1-Q)^{(n-1)}\right] \geq \frac{(n-1)Q}{1+(n-1)Q} \tag{3.19}$$

This gives

$$\langle W_R\rangle_0 \;\geq\; \frac{n(n-1)}{\nu(R)} \cdot \frac{Q}{1+(n-1)Q}, \tag{3.20}$$

$$\langle W_R\rangle_0 \;\leq\; \frac{n(n-1)}{\nu(R)} \cdot Q\ . \tag{3.21}$$

From Temple's inequality [T] we obtain like in (2.38) the estimate

$$E_0(n,\ell) \geq (1-\varepsilon)\langle W_R\rangle_0 \left(1 - \frac{\mu\big(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2\big)}{\langle W_R\rangle_0\big(E_1^{(0)} - \mu\langle W_R\rangle_0\big)}\right) \tag{3.22}$$

where

$$E_1^{(0)} = \frac{\varepsilon\mu}{\ell^2} \tag{3.23}$$

is the energy of the lowest excited state of εT_n. This estimate is valid for $E_1^{(0)}/\mu > \langle W_R\rangle_0$, i.e., it is important that ℓ is not too big.

Putting (3.20)–(3.22) together we obtain the estimate

$$E_0(n,\ell) \geq \frac{n(n-1)}{\ell^2}\,\frac{A(R)}{\nu(R)}\,K(n) \tag{3.24}$$

with

$$K(n) = (1-\varepsilon)\cdot \frac{(1-\frac{2R}{\ell})^2}{1+(n-1)Q} \cdot \left(1 - \frac{n}{(\varepsilon\,\nu(R)/\ell^2) - n(n-1)\,Q}\right) \tag{3.25}$$

Note that Q depends on ℓ and R, and K depends on ℓ, R and ε besides n. We have here dropped the term $\langle W_R\rangle_0^2$ in the numerator in (3.22), which is appropriate for the purpose of a lower bound.

We note that K is monotonically decreasing in n, so for a given n we may replace $K(n)$ by $K(p)$ provided $p \geq n$. As explained in the previous section, (2.45)–(2.52), convexity of $n \mapsto n(n-1)$ together with superadditivity of $E_0(n,\ell)$ in n leads, for $p = 4\rho\ell^2$, to an estimate for the energy of N particles in the large box when the side length L is an integer multiple of ℓ:

$$E_0(N,L)/N \geq \frac{\rho A(R)}{\nu(R)}\left(1 - \frac{1}{\rho\ell^2}\right) K(4\rho\ell^2) \tag{3.26}$$

with $\rho = N/L^2$.

Let us now look at the conditions on the parameters ε, R and ℓ that have to be met in order to obtain a lower bound with the same leading term as the upper bound (3.3).

From (3.13) we have

$$\frac{A(R)}{\nu(R)} = \frac{4\pi}{(\ln(R^2/a^2)-1)}\big(1 - \mathrm{O}((R_0^2/R^2)\ln(R/R_0)\big) \tag{3.27}$$

We thus see that as long as $a < R < \rho^{-1/2}$ the logarithmic factor in the denominator in (3.27) has the right form for a lower bound. Moreover, for Temple's inequality the denominator in the third factor in (3.25) must be positive. With $n = 4\rho\ell^2$ and $\nu(R) \geq (\text{const.}) R^2 \ln(R^2/a^2)$ for $R \gg R_0$, this condition amounts to

$$(\text{const.})\varepsilon \ln(R^2/a^2)/\ell^2 > \rho^2\ell^4. \tag{3.28}$$

The relative error terms in (3.26) that have to be $\ll 1$ are

$$\varepsilon, \quad \frac{1}{\rho\ell^2}, \quad \frac{R}{\ell}, \quad \rho R^2, \quad \frac{\rho\ell^4}{\varepsilon R^2 \ln(R^2/a^2)}. \tag{3.29}$$

We now choose

$$\varepsilon \sim |\ln(\rho a^2)|^{-1/5}, \quad \ell \sim \rho^{-1/2}|\ln(\rho a^2)|^{1/10}, \quad R \sim \rho^{-1/2}|\ln(\rho a^2)|^{-1/10} \tag{3.30}$$

Condition (3.28) is satisfied since the left side is $> (\text{const.})|\ln(\rho a^2)|^{3/5}$ and the right side is $\sim |\ln(\rho a^2)|^{2/5}$. The first three error terms in (3.29) are all of the same order, $|\ln(\rho a^2)|^{-1/5}$, the last is $\sim |\ln(\rho a^2)|^{-1/5}(\ln|\ln(\rho a^2)|)^{-1}$. With these choices, (3.26) thus leads to the following:

Theorem 3.3 (Lower bound). *For all N and L large enough such that $L > (\text{const.})\rho^{-1/2}|\ln(\rho a^2)|^{1/10}$ and $N > (\text{const.})|\ln(\rho a^2)|^{1/5}$ with $\rho = N/L^2$, the ground state energy with Neumann boundary condition satisfies*

$$E_0(N,L)/N \geq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}\left(1 - \mathrm{O}(|\ln(\rho a^2)|^{-1/5})\right). \tag{3.31}$$

In combination with the upper bound (3.3) this also proves

Theorem 3.4 (Energy at low density in the thermodynamic limit).

$$\lim_{\rho a^2 \to 0} \frac{e_0(\rho)}{4\pi\mu\rho|\ln(\rho a^2)|^{-1}} = 1 \tag{3.32}$$

where $e_0(\rho) = \lim_{N\to\infty} E_0(N, \rho^{-1/2}N^{1/2})/N$. This holds irrespective of boundary conditions.

As in the three-dimensional case, Theorem 3.4 is also valid for an infinite range potential v provided that $v \geq 0$ and for some R we have $\int_R^\infty v(r)r\,dr < \infty$, which guarantees a finite scattering length.

4. Bose-Einstein Condensation

Let us now comment on the notion of Bose-Einstein condensation (BEC). Given the normalized ground state wave function $\Psi_0(\vec{x}_1,\ldots,\vec{x}_N)$ we can form the one-body density matrix which is an operator on $L^2(\mathbb{R}^d)$ ($d = 2$ or 3) given by the kernel

$$\gamma(\vec{x},\vec{x}') = N\int \Psi_0(\vec{x},\vec{X})\Psi_0(\vec{x}',\vec{X})d\vec{X}\ , \tag{4.1}$$

where we introduced the short hand notation

$$\vec{X} = (\vec{x}_2, \ldots, \vec{x}_N) \qquad \text{and} \quad d\vec{X} = \prod_{j=2}^{N} d\vec{x}_j. \tag{4.2}$$

Then $\int \gamma(\vec{x}, \vec{x})d\vec{x} = \mathrm{Tr}\,[\gamma] = N$. BEC in the ground state is the assertion that this operator has an eigenvalue of order N in the thermodynamic limit. Since γ is a positive kernel and, hopefully, translation invariant in the thermodynamic limit, the eigenfunction belonging to the largest eigenvalue must be the constant function $L^{-d/2}$. Therefore, another way to say that there is BEC in the ground state is that

$$\frac{1}{L^d} \int\int \gamma(\vec{x}, \vec{y})d\vec{x}d\vec{y} = \mathrm{O}(N) \tag{4.3}$$

as $N \to \infty$, $L \to \infty$ with N/L^d fixed. Unfortunately, this is something that is frequently invoked but never proved for many body Hamiltonians with genuine interactions — except for one special case: hard core bosons on a lattice at half-filling (i.e., N = half the number of lattice sites). The proof is in [KLS].

The problem remains open after more than 75 years since the first investigations on the Bose gas [B, E]. It is also not at all clear that BEC is essential for superfluidity, as frequently claimed. Our construction in Section 2 shows that (in 3D) BEC exists on a length scale of order $\rho^{-1/3}Y^{-1/17}$ which, unfortunately, is not a 'thermodynamic' length like volume$^{1/3}$. The same remark applies to the 2D case of Section 3, where BEC is proved over a length scale $\rho^{-1/10}|\ln(\rho a^2)|^{1/10}$.

In a certain *dilute* limit, however, one can prove (4.3), as has been recently shown in [LSe]. In this limit the interaction potential v is varied with N so that the ratio a/L of the scattering length to the box length is of order $1/N$. In [LSe] the case of a Bose gas confined in an external trap potential was considered (see Sections 5 and 6), but the analysis for a homogeneous gas is even simpler and implies the following result. For simplicity, we shall treat only the 3D case.

Theorem 4.1 (BEC in a dilute limit). *Assume that, as $N \to \infty$, $\rho = N/L^3$ and $g = Na/L$ stay fixed, and impose either periodic or Neumann boundary conditions for H. Then*

$$\lim_{N\to\infty} \frac{1}{N}\frac{1}{L^3} \int\int \gamma(\vec{x}, \vec{y})d\vec{x}d\vec{y} = 1 \ . \tag{4.4}$$

The reason why the limit $N \to \infty$ with Na/L fixed is particularly interesting will become clear when we study systems confined in a trap potential in the next section. Note that the limit we consider is really a limit of a *dilute* gas, since

$$a^3\rho = \left(\frac{Na}{L}\right)^3 \frac{1}{N^2} = O(N^{-2})$$

as $N \to \infty$. Since the ground state energy is of the order $a\rho \sim L^{-2}$ is this limit, it is also clear why we do not deal with Dirichlet boundary conditions: there would be an additional contribution to the energy of the same order, and the system would not be homogeneous any more. Dirichlet boundary conditions can, however, be treated with the methods of Section 6.

At this point we should say what we mean exactly by changing a with N. We do this by scaling, i.e., we write

$$v(|\vec{x}|) = \frac{1}{a^2} v_1(|\vec{x}|/a) \tag{4.5}$$

for some v_1 having scattering length 1, and vary a while keeping v_1 fixed. It is easily checked that the v so defined has scattering length a. It is important to note that, in the limit considered, a tends to zero (as $N^{-2/3}$), and v becomes a *hard* potential of *short* range. This is the *opposite* of the usual mean field limit where the strength of the potential goes to zero while its range tends to infinity.

Proof of Theorem 4.1. Let $g = Na/L$ and $\rho = N/L^3$ be fixed as $N \to \infty$. Since $a^3\rho \to 0$, Theorems 2.2 and 2.4 imply

$$\begin{aligned}\lim_{N\to\infty} \left(\frac{N}{\rho}\right)^{2/3} \int d\vec{X} d\vec{x}_1 \Bigg(\mu |\nabla_{\vec{x}_1} \Psi_0(\vec{x}_1, \vec{X})|^2 \\ + \tfrac{1}{2} \sum_{j=2}^{N} v(|\vec{x}_1 - \vec{x}_j|) |\Psi_0(\vec{x}_1, \vec{X})|^2 \Bigg) = 4\pi\mu g,\end{aligned} \tag{4.6}$$

where we again used the short hand notation (4.2). The symmetry of Ψ_0 and the boundary conditions have also been used. Even more is true, namely that

$$\lim_{N\to\infty} \left(\frac{N}{\rho}\right)^{2/3} \int d\vec{X} d\vec{x}_1 \mu |\nabla_{\vec{x}_1} \Psi_0(\vec{x}_1, \vec{X})|^2 = 4\pi\mu g s \tag{4.7}$$

and

$$\lim_{N\to\infty} \left(\frac{N}{\rho}\right)^{2/3} \int d\vec{X} d\vec{x}_1 \tfrac{1}{2} \sum_{j=2}^{N} v(|\vec{x}_1 - \vec{x}_j|) |\Psi_0(\vec{x}_1, \vec{X})|^2 = 4\pi\mu g (1-s) \tag{4.8}$$

for some $0 < s \leq 1$. The parameter s is given by $s = \int |\nabla\psi_0|^2/(4\pi a)$, where ψ_0 denotes the solution to the scattering equation for v (under the boundary condition $\lim_{|\vec{x}|\to\infty} \psi_0(\vec{x}) = 1$; see Eq. (2.3)). This is a simple consequence of (4.6) by variation with respect to the different components of the energy, as was also noted in [CS2]. More precisely, the ground state energy is a concave function of the mass parameter μ, so it is legitimate to differentiate both sides of (4.6) with respect to μ. In doing so, it has to be noted that g depends on μ through the scattering length. Using (2.13) one sees that

$$\frac{d(\mu a)}{d\mu} = \frac{1}{4\pi} \int |\nabla\psi_0|^2 d\vec{x} \tag{4.9}$$

by the Feynman-Hellmann principle, since ψ_0 minimizes the left side of (2.13).

We now concentrate on the term (4.7) and show that to leading order all the energy is located in small balls surrounding each particle. These balls can be taken to have radius roughly $N^{-4/51}$ compared to the mean particle distance $\rho^{-1/3}$. More precisely, we will show that

$$\lim_{N\to\infty} N^{2/3}\int d\vec{X}\int_{\Omega_{\vec{X}}} d\vec{x}_1 |\nabla_{\vec{x}_1}\Psi_0(\vec{x}_1,\vec{X})|^2 = 0\ , \tag{4.10}$$

where, for fixed $\vec{X}$, $\Omega_{\vec{X}}$ is given by

$$\Omega_{\vec{X}} = \left\{\vec{x}\in\Lambda\,\middle|\,\min_{k\geq 2}|\vec{x}-\vec{x}_k|\geq N^{-4/51}\right\}\ . \tag{4.11}$$

To see this, we shall show that (4.6) still holds true if the integrals in the first term are restricted to the complement of $\Omega_{\vec{X}}$, denoted by $\Omega^c_{\vec{X}}$. The proof of this is actually just a detailed examination of the lower bounds to the ground state energy derived in Subsection 2.2. What we have to show is

$$\sum_{i=1}^N \int_{\Omega_i^c}\mu|\nabla_i\Psi_0|^2 d\vec{x}_1 d\vec{X} + \sum_{i<j}\int v(|\vec{x}_i-\vec{x}_j|)|\Psi_0|^2 d\vec{x}_1 d\vec{X} \geq 4\pi\mu a\rho N(1-o(1)) \tag{4.12}$$

as $N\to\infty$, where Ω_i^c denotes the set

$$\Omega_i^c = \{(\vec{x}_1,\vec{X})\in\Lambda^N|\ \min_{k\neq i}|\vec{x}_i-\vec{x}_k|\leq N^{-4/51}\}\ .$$

While (4.12) is not true for all conceivable Ψ's satisfying the normalization condition $\|\Psi\|_2 = 1$, it *is* true for Ψ_0. Namely, we claim that

$$\begin{aligned}\sum_{i=1}^N\left(\int_{\Omega_i^c}\mu|\nabla_i\Psi|^2 d\vec{x}_1 d\vec{X} + \varepsilon\int|\nabla_i\Psi|^2 d\vec{x}_1 d\vec{X}\right)&\\ +\sum_{i<j}\int v(|\vec{x}_i-\vec{x}_j|)|\Psi|^2 d\vec{x}_1 d\vec{X} \geq 4\pi\mu a\rho N(1-o(1))&\end{aligned} \tag{4.13}$$

for any Ψ, as long as $\varepsilon\geq O(N^{-2/17})$ as $N\to\infty$. Since (4.7) implies that Ψ_0 has total kinetic energy of order $O(a\rho N) = O(N^{1/3})$, (4.12) follows from (4.13).

It remains to prove (4.13), but this has essentially already been done in Subsection 2.2! Namely, the usage of the Dyson Lemma 2.5 requires only the kinetic energy inside balls of radius $R = O(N^{-4/51})$ around each particle. In fact, by Eqs.(2.56) and (2.57), $R\sim aY^{-5/17}$ with $Y\sim a^3\rho\sim N^{-2}$ and $a\sim N^{-2/3}$ (the latter because $g = Na/L$ is fixed and $L\sim N^{1/3}$). The second term in (4.13), the total kinetic energy multiplied by ε, together with the 'softened' potential (2.30), then gives the desired lower bound to the energy (see (2.35)–(2.39)), as long as $\varepsilon\geq O(N^{-2/17})$. This proves (4.13) with an error term of the order $O(N^{-2/17})$, and therefore also (4.12) with a relative error $O(N^{-2/17})$.

Eq. (4.10) means that $\nabla_{\vec{x}}\Psi_0(\vec{x},\vec{X})$ is almost zero (in an L^2 sense) outside of the small balls $\Omega^c_{\vec{X}}$. To conclude BEC we need to show that as a function of $\vec{x}$, $\Psi_0(\vec{x},\vec{X})$ is essentially constant in $\Omega_{\vec{X}}$. Although $\Omega_{\vec{X}}$ has a big volume, it can be a weird, and even disconnected, set, so this conclusion is not yet possible. However, exploiting the knowledge that the *total* kinetic energy of Ψ_0 (including the balls) is not huge (see (4.7)), we an show the desired constancy of Ψ_0. What we need for this purpose is the following special case of the generalized Poincaré inequality that will be stated more generally in Lemma 6.5 in Section 6.

Lemma 4.2 **(Generalized Poincaré inequality, special case).** *Let $\Lambda \subset \mathbb{R}^3$ be a cube of side length L, and define the average of a function $f \in L^1(\Lambda)$ by*

$$\langle f\rangle_\Lambda = \frac{1}{L^3}\int_\Lambda f(\vec{x})\,d\vec{x}\ .$$

There exists a constant C such that for all measurable sets $\Omega \subset \Lambda$ and all $f \in H^1(\Lambda)$ the inequality

$$\int_\Lambda |f(\vec{x}) - \langle f\rangle_\Lambda|^2 d\vec{x} \le C\left(L^2\int_\Omega |\nabla f(\vec{x})|^2 d\vec{x} + |\Omega^c|^{2/3}\int_\Lambda |\nabla f(\vec{x})|^2 d\vec{x}\right) \tag{4.14}$$

holds. Here $\Omega^c = \Lambda\setminus\Omega$, and $|\cdot|$ denotes the measure of a set. .

Proof. By scaling, it suffices to consider the case $L = 1$. Using the usual Poincaré-Sobolev inequality on Λ (see [LLo], Thm. 8.12), we infer that there exists a $C > 0$ such that

$$\begin{aligned}\|f - \langle f\rangle_\Lambda\|^2_{L^2(\Lambda)} &\le \tfrac{1}{2}C\|\nabla f\|^2_{L^{6/5}(\Lambda)}\\ &\le C\left(\|\nabla f\|^2_{L^{6/5}(\Omega)} + \|\nabla f\|^2_{L^{6/5}(\Omega^c)}\right)\ .\end{aligned} \tag{4.15}$$

Applying Hölder's inequality

$$\|\nabla f\|_{L^{6/5}(\Omega)} \le \|\nabla f\|_{L^2(\Omega)}|\Omega|^{1/3}$$

(and the analogue with Ω replaced by Ω^c), we see that (4.14) holds. ∎

Applying this result, we are now able to finish the proof of Theorem 4.1. Denote by $\langle\Psi_0\rangle_{\Lambda,\vec{X}}$ the average of $\Psi_0(\vec{x},\vec{X})$ over $\vec{x}\in\Lambda$. Using Lemma 4.2, with $\Omega = \Omega_{\vec{X}}$ and $f(\vec{x}) = \Psi_0(\vec{x}, \vec{X}) - \langle \Psi_0 \rangle_{\Lambda, \vec{X}}$, we conclude that

$$\begin{aligned} &\int d\vec{X} \int d\vec{x} \left[\Psi_0(\vec{x}, \vec{X}) - \langle \Psi_0 \rangle_{\Lambda, \vec{X}} \right]^2 \\ &\leq C \int d\vec{X} \left[L^2 \int_{\Omega_{\vec{X}}} |\nabla_{\vec{x}} \Psi_0(\vec{x}, \vec{X})|^2 d\vec{x} \right. \\ &\qquad \left. + \left(\frac{4\pi}{3} \right)^{2/3} N^{2/3 - 8/51} \int_\Lambda |\nabla_{\vec{x}} \Psi_0(\vec{x}, \vec{X})|^2 d\vec{x} \right], \quad (4.16) \end{aligned}$$

where we used that $|\Omega^c_{\vec{X}}| \leq (4\pi/3) N^{1-4/17}$. The first integral on the right side of (4.16) tends to zero as $N \to \infty$ by (4.10), and the second term vanishes in this limit because of (4.7). Moreover,

$$\begin{aligned} &\int \int d\vec{X} d\vec{x} \left[\Psi_0(\vec{x}, \vec{X}) - \langle \Psi_0 \rangle_{\Lambda, \vec{X}} \right]^2 \\ &= \int \int d\vec{X} d\vec{x} |\Psi_0(\vec{x}, \vec{X})|^2 - \frac{1}{N} \frac{1}{L^3} \int \int \gamma(\vec{x}, \vec{y}) d\vec{x} d\vec{y} \ . \quad (4.17) \end{aligned}$$

We conclude that

$$\liminf_{N \to \infty} \frac{1}{N} \frac{1}{L^3} \int \int \gamma(\vec{x}, \vec{y}) d\vec{x} d\vec{y} \geq \lim_{N \to \infty} \int \int d\vec{X} d\vec{x} |\Psi_0(\vec{x}, \vec{X})|^2 = 1 \ , \quad (4.18)$$

and Theorem 4.1 is proven. ■

As stated, Theorem 4.1 is concerned with a simultaneous thermodynamic and $a \to 0$ limit, where, as $N \to \infty$, the box length L is proportional to $N^{1/3}$ and $a \sim N^{-2/3}$. By scaling, the above result is equivalent to considering a Bose gas in a *fixed box* of side length $L = 1$, and keeping Na fixed as $N \to \infty$, i.e., $a \sim 1/N$. The ground state energy of the system is then, asymptotically, $N \times 4\pi N a$, and Theorem 4.1 implies that the one-particle reduced density matrix γ of the ground state converges, after division by N, to the projection onto the constant function. An analogous result holds true for inhomogeneous systems. This was recently shown in [LSe] and will be presented in Section 6.

5. Gross-Pitaevskii Equation for Trapped Bosons

In the recent experiments on Bose condensation (see, e.g., [KD]), the particles are confined at very low temperatures in a 'trap' where the particle density is *inhomogeneous*, contrary to the case of a large 'box', where the density is essentially uniform. We model the trap by a slowly varying confining potential V, with $V(\vec{x}) \to \infty$ as $|\vec{x}| \to \infty$. The Hamiltonian becomes

$$H = \sum_{i=1}^N \{ -\mu \Delta_i + V(\vec{x}_i) \} + \sum_{1 \leq i < j \leq N} v(|\vec{x}_i - \vec{x}_j|) \ . \quad (5.1)$$

Shifting the energy scale if necessary we can assume that V is nonnegative. The ground state energy, $\hbar\omega$, of $-\mu\Delta + V(\vec{x})$ is a natural energy unit and the corresponding length unit, $\sqrt{\hbar/(m\omega)} = \sqrt{2\mu/(\hbar\omega)} \equiv L_{\rm osc}$, is a measure of the extension of the trap.

In the sequel we shall be considering a limit where $a/L_{\rm osc}$ tends to zero while $N \to \infty$. Experimentally $a/L_{\rm osc}$ can be changed in two ways: One can either vary $L_{\rm osc}$ or a. The first alternative is usually simpler in practice but very recently a direct tuning of the scattering length itself has also been shown to be feasible [CCRCW]. Mathematically, both alternatives are equivalent, of course. The first corresponds to writing $V(\vec{x}) = L_{\rm osc}^{-2} V_1(\vec{x}/L_{\rm osc})$ and keeping V_1 and v fixed. The second corresponds to writing the interaction potential as $v(|\vec{x}|) = a^{-2} v_1(|\vec{x}|/a)$ like in (4.5), where v_1 has unit scattering length, and keeping V and v_1 fixed. This is equivalent to the first, since for given V_1 and v_1 the ground state energy of (5.1), measured in units of $\hbar\omega$, depends only on N and $a/L_{\rm osc}$. In the dilute limit when a is much smaller than the mean particle distance, the energy becomes independent of v_1.

We choose $L_{\rm osc}$ as a length unit. The energy unit is $\hbar\omega = 2\mu L_{\rm osc}^{-2} = 2\mu$. Moreover, we find it convenient to regard V and v_1 as fixed. This justifies the notion $E_0(N, a)$ for the quantum mechanical ground state energy.

The idea is now to use the information about the thermodynamic limiting energy of the dilute Bose gas in a box to find the ground state energy of (5.1) in an appropriate limit. This has been done in [LSeY1, LSeY2] and in this section we give an account of this work. As we saw in Sections 2 and 3 there is a difference in the ρ dependence between two and three dimensions, so we can expect a related difference now. We discuss 3D first.

5.1. **Three Dimensions.** Associated with the quantum mechanical ground state energy problem is the Gross-Pitaevskii (GP) energy functional [G1, G2, Pi]

$$\mathcal{E}^{\rm GP}[\phi] = \int_{\mathbb{R}^3} \left(\mu |\nabla\phi|^2 + V|\phi|^2 + 4\pi\mu a|\phi|^4 \right) d\vec{x} \tag{5.2}$$

with the subsidiary condition

$$\int_{\mathbb{R}^3} |\phi|^2 = N. \tag{5.3}$$

As before, $a > 0$ is the scattering length of v. The corresponding energy is

$$E^{\rm GP}(N, a) = \inf_{\int|\phi|^2 = N} \mathcal{E}^{\rm GP}[\phi] = \mathcal{E}^{\rm GP}[\phi^{\rm GP}], \tag{5.4}$$

with a unique, positive $\phi^{\rm GP}$. The existence of the minimizer $\phi^{\rm GP}$ is proved by standard techniques and it can be shown to be continuously differentiable, see [LSeY1], Sect. 2 and Appendix A. The minimizer depends on N and a, of course, and when this is important we denote it by $\phi^{\rm GP}_{N,a}$.

The variational equation satisfied by the minimizer is the *GP equation*

$$-\mu\Delta\phi^{\rm GP}(\vec{x}) + V(\vec{x})\phi^{\rm GP}(\vec{x}) + 8\pi\mu a \phi^{\rm GP}(\vec{x})^3 = \mu^{\rm GP}\phi^{\rm GP}(\vec{x}), \tag{5.5}$$

where μ^{GP} is the chemical potential, given by

$$\mu^{\mathrm{GP}} = dE^{\mathrm{GP}}(N,a)/dN = E^{\mathrm{GP}}(N,a)/N + (4\pi\mu a/N)\int |\phi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x}. \tag{5.6}$$

The GP theory has the following scaling property:

$$E^{\mathrm{GP}}(N,a) = NE^{\mathrm{GP}}(1,Na), \tag{5.7}$$

and

$$\phi^{\mathrm{GP}}_{N,a}(\vec{x}) = N^{1/2}\phi^{\mathrm{GP}}_{1,Na}(\vec{x}). \tag{5.8}$$

Hence we see that the relevant parameter in GP theory is the combination Na.

We now turn to the relation of E^{GP} and ϕ^{GP} to the quantum mechanical ground state. If $v = 0$, then the ground state of (5.1) is

$$\Psi_0(\vec{x}_1,\ldots,\vec{x}_N) = \textstyle\prod_{i=1}^N \phi_0(\vec{x}_i)$$

with ϕ_0 the normalized ground state of $-\mu\Delta + V(\vec{x})$. In this case clearly $\phi^{\mathrm{GP}} = \sqrt{N}\ \phi_0$, and then $E^{\mathrm{GP}} = N\hbar\omega = E_0$. In the other extreme, if $V(\vec{x}) = 0$ for $\vec{x}$ inside a large box of volume L^3 and $V(\vec{x}) = \infty$ otherwise, then $\phi^{\mathrm{GP}} \approx \sqrt{N/L^3}$ and we get $E^{\mathrm{GP}}(N,a) = 4\pi\mu a N^2/L^3$, which is the previously considered energy E_0 for the homogeneous gas in the low density regime. (In this case, the gradient term in $\mathcal{E}^{\mathrm{GP}}$ plays no role.)

In general, we expect that for *dilute* gases in a suitable limit

$$E_0 \approx E^{\mathrm{GP}} \quad \text{and} \quad \rho^{\mathrm{QM}}(\vec{x}) \approx \left|\phi^{\mathrm{GP}}(\vec{x})\right|^2 \equiv \rho^{\mathrm{GP}}(\vec{x}), \tag{5.9}$$

where the quantum mechanical particle density in the ground state is defined by

$$\rho^{\mathrm{QM}}(\vec{x}) = N\int |\Psi_0(\vec{x},\vec{x}_2,\ldots,\vec{x}_N)|^2 d\vec{x}_2\cdots d\vec{x}_N. \tag{5.10}$$

Dilute means here that

$$\bar{\rho}a^3 \ll 1, \tag{5.11}$$

where

$$\bar{\rho} = \frac{1}{N}\int |\rho^{\mathrm{GP}}(\vec{x})|^2 d\vec{x} \tag{5.12}$$

is the *mean density.*

The limit in which (5.9) can be expected to be true should be chosen so that *all three* terms in $\mathcal{E}^{\mathrm{GP}}$ make a contribution. The scaling relations (5.7) and (5.8) indicate that fixing Na as $N \to \infty$ is the right thing to do (and this is quite relevant since experimentally N can be quite large, 10^6 and more, and Na can range from about 1 to 10^4 [DGPS]). Fixing Na (which we refer to as the GP case) also means that we really are dealing with a dilute limit, because the mean density $\bar{\rho}$ is then of the order N (since $\bar{\rho}_{N,a} = N\bar{\rho}_{1,Na}$) and hence

$$a^3\bar{\rho} \sim N^{-2}. \tag{5.13}$$

The precise statement of (5.9) is:

Theorem 5.1 (GP limit of the QM ground state energy and density). *If $N \to \infty$ with Na fixed, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\rm GP}(N,a)} = 1, \tag{5.14}$$

and

$$\lim_{N\to\infty} \frac{1}{N}\rho^{\rm QM}_{N,a}(\vec{x}) = \left|\phi^{\rm GP}_{1,Na}(\vec{x})\right|^2 \tag{5.15}$$

in the weak L^1-sense.

To describe situations where Na is very large, it is appropriate to consider a limit where, as $N \to \infty$, $a \gg N^{-1}$, i.e. $Na \to \infty$, but still $\bar{\rho}a^3 \to 0$. In this case, the gradient term in the GP functional becomes negligible compared to the other terms and the so-called *Thomas-Fermi (TF) functional*

$$\mathcal{E}^{\rm TF}[\rho] = \int_{\mathbb{R}^3} \left(V\rho + 4\pi\mu a\rho^2\right) d\vec{x} \tag{5.16}$$

arises. (Note that this functional has nothing to do with the fermionic theory invented by Thomas and Fermi in 1927, except for a certain formal analogy.) It is defined for nonnegative functions ρ on $\mathbb{R}^3$. Its ground state energy $E^{\rm TF}$ and density $\rho^{\rm TF}$ are defined analogously to the GP case. (The TF functional is especially relevant for the two-dimensional Bose gas. There a has to decrease exponentially with N in the GP limit, so the TF limit is more adequate; see Subsection 5.2 below).

Our second main result of this section is that minimization of (5.16) reproduces correctly the ground state energy and density of the many-body Hamiltonian in the limit when $N \to \infty$, $a^3\bar{\rho} \to 0$, but $Na \to \infty$ (which we refer to as the TF case), provided the external potential is reasonably well behaved. We will assume that V is asymptotically equal to some function W that is homogeneous of some order $s > 0$, i.e., $W(\lambda\vec{x}) = \lambda^s W(\vec{x})$ for all $\lambda > 0$, and locally Hölder continuous (see [LSeY2] for a precise definition). This condition can be relaxed, but it seems adequate for most practical applications and simplifies things considerably.

Theorem 5.2 (TF limit of the QM ground state energy and density). *Assume that V satisfies the conditions stated above. If $g \equiv Na \to \infty$ as $N \to \infty$, but still $a^3\bar{\rho} \to 0$, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\rm TF}(N,a)} = 1, \tag{5.17}$$

and

$$\lim_{N\to\infty} \frac{g^{3/(s+3)}}{N} \rho^{\rm QM}_{N,a}(g^{1/(s+3)}\vec{x}) = \tilde{\rho}^{\rm TF}_{1,1}(\vec{x}) \tag{5.18}$$

in the weak L^1-sense, where $\tilde{\rho}^{\rm TF}_{1,1}$ is the minimizer of the TF functional under the condition $\int \rho = 1$, $a = 1$, and with V replaced by W.

In the following, we will present the essentials of the proofs Theorems 5.1 and 5.2. We will derive appropriate upper and lower bounds on the ground state energy E_0.

The proof of the lower bound in Theorem 5.1 presented here is a modified version of (and partly simpler than) the original proof in [LSeY1].

The convergence of the densities follows from the convergence of the energies in the usual way by variation with respect to the external potential. For simplicity, we set $\mu \equiv 1$ in the following.

Proof of Theorems 5.1 and 5.2. Part 1: Upper bound to the QM energy. To derive an upper bound on E_0 we use a generalization of a trial wave function of Dyson [D1], who used this function to give an upper bound on the ground state energy of the homogeneous hard core Bose gas (c.f. Section 2.1). It is of the form

$$\Psi(\vec{x}_1,\ldots,\vec{x}_N) = \prod_{i=1}^N \phi^{\rm GP}(\vec{x}_i) F(\vec{x}_1,\ldots,\vec{x}_N), \tag{5.19}$$

where F is constructed in the following way:

$$F(\vec{x}_1,\ldots,\vec{x}_N) = \prod_{i=1}^N f(t_i(\vec{x}_1,\ldots,\vec{x}_i)), \tag{5.20}$$

where $t_i = \min\{|\vec{x}_i - \vec{x}_j|, 1 \le j \le i-1\}$ is the distance of $\vec{x}_i$ to its *nearest neighbor* among the points $\vec{x}_1,\ldots,\vec{x}_{i-1}$, and f is a function of $r \ge 0$. As in (2.20) we choose it to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } \ r < b \\ 1 & \text{for } \ r \ge b, \end{cases} \tag{5.21}$$

where f_0 is the solution of the zero energy scattering equation (2.3) and b is some cut-off parameter of order $b \sim \bar{\rho}^{-1/3}$. The function (5.19) is not totally symmetric, but for an upper bound it is nevertheless an acceptable test wave function since the bosonic ground state energy is equal to the *absolute* ground state energy.

The result of a somewhat lengthy computation (see [LSeY1] for details) is the upper bound

$$E_0(N,a) \le E^{\rm GP}(N,a)\left(1 + O(a\bar{\rho}^{1/3})\right). \tag{5.22}$$

Part 2: Lower bound to the QM energy, GP case. To obtain a lower bound for the QM ground state energy the strategy is to divide space into boxes and use the estimate on the homogeneous gas, given in Theorem 2.4, in each box with *Neumann* boundary conditions. One then minimizes over all possible divisions of the particles among the different boxes. This gives a lower bound to the energy because discontinuous wave functions for the quadratic form defined by the Hamiltonian are now allowed. We can neglect interactions among particles in different boxes because $v \geq 0$. Finally, one lets the box size tend to zero. However, it is not possible to simply approximate V by a constant potential in each box. To see this consider the case of noninteracting particles, i.e., $v = 0$ and hence $a = 0$. Here $E_0 = N\hbar\omega$, but a 'naive' box method gives only $\min_{\vec{x}} V(\vec{x})$ as lower bound, since it clearly pays to put all the particles with a constant wave function in the box with the lowest value of V.

For this reason we start by separating out the GP wave function in each variable and write a general wave function Ψ as

$$\Psi(\vec{x}_1,\dots,\vec{x}_N) = \prod_{i=1}^N \phi^{\rm GP}(\vec{x}_i)F(\vec{x}_1,\dots,\vec{x}_N). \tag{5.23}$$

Here $\phi^{\rm GP} = \phi^{\rm GP}_{N,a}$ is normalized so that $\int|\phi^{\rm GP}|^2 = N$. Eq. (5.23) defines F for a given Ψ because $\phi^{\rm GP}$ is everywhere strictly positive, being the ground state of the operator $-\Delta+V+8\pi a|\phi^{\rm GP}|^2$. We now compute the expectation value of H in the state Ψ. Using partial integration and the variational equation (5.5) for $\phi^{\rm GP}$, we see that

$$\frac{\langle\Psi|H\Psi\rangle}{\langle\Psi|\Psi\rangle} - E^{\rm GP}(N,a) = 4\pi a\int|\rho^{\rm GP}|^2 + Q(F), \tag{5.24}$$

with

$$Q(F) = \sum_{i=1}^N \frac{\int\prod_{k=1}^N \rho^{\rm GP}(\vec{x}_k)\left(|\nabla_i F|^2 + \frac{1}{2}\sum_{j\neq i} v(|\vec{x}_i-\vec{x}_j|)|F|^2 - 8\pi a\rho^{\rm GP}(\vec{x}_i)|F|^2\right)}{\int\prod_{k=1}^N \rho^{\rm GP}(\vec{x}_k)|F|^2}. \tag{5.25}$$

We recall that $\rho^{\rm GP}(\vec{x}) = |\phi^{\rm GP}_{N,a}(\vec{x})|^2$. For computing the ground state energy of H we have to minimize the normalized quadratic form Q. Compared to the expression for the energy involving Ψ itself we have thus obtained the replacements

$$V(\vec{x}) \to -8\pi a\rho^{\rm GP}(\vec{x}) \quad \text{and} \quad \prod_{i=1}^N d\vec{x}_i \to \prod_{i=1}^N \rho^{\rm GP}(\vec{x}_i)d\vec{x}_i\ . \tag{5.26}$$

We now use the box method on *this* problem. More precisely, labeling the boxes by an index α, we have

$$\inf_F Q(F) \geq \inf_{\{n_\alpha\}} \sum_\alpha \inf_{F_\alpha} Q_\alpha(F_\alpha), \tag{5.27}$$

where Q_α is defined by the same formula as Q but with the integrations limited to the box α, F_α is a wave function with particle number n_α, and the infimum is taken over all distributions of the particles with $\sum n_\alpha = N$.

We now fix some $M > 0$, that will eventually tend to ∞, and restrict ourselves to boxes inside a cube Λ_M of side length M. Since $v \geq 0$ the contribution to (5.27) of boxes outside this cube is easily estimated from below by $-8\pi Na \sup_{\vec{x}\notin\Lambda_M} \rho^{\rm GP}(\vec{x})$, which, divided by N, is arbitrarily small for M large, since Na is fixed and $\phi^{\rm GP}/N^{1/2} = \phi^{\rm GP}_{1,Na}$ decreases faster than exponentially at infinity ([LSeY1], Lemma A.5).

For the boxes inside the cube Λ_M we want to use Lemma 2.5 and therefore we must approximate $\rho^{\rm GP}$ by constants in each box. Let $\rho_{\alpha,\max}$ and $\rho_{\alpha,\min}$, respectively, denote the maximal and minimal values of $\rho^{\rm GP}$ in box α. Define

$$\Psi_\alpha(\vec{x}_1,\dots,\vec{x}_{n_\alpha}) = F_\alpha(\vec{x}_1,\dots,\vec{x}_{n_\alpha}) \prod_{k=1}^{n_\alpha} \phi^{\rm GP}(\vec{x}_k), \tag{5.28}$$

and

$$\Psi_\alpha^{(i)}(\vec{x}_1,\dots,\vec{x}_{n_\alpha}) = F_\alpha(\vec{x}_1,\dots,\vec{x}_{n_\alpha}) \prod_{\substack{k=1\\k\neq i}}^{n_\alpha} \phi^{\rm GP}(\vec{x}_k). \tag{5.29}$$

We have, for all $1 \leq i \leq n_\alpha$,

$$\begin{aligned}&\int \prod_{k=1}^{n_\alpha} \rho^{\rm GP}(\vec{x}_k)\left(|\nabla_i F_\alpha|^2 + \tfrac12 \sum_{j\neq i} v(|\vec{x}_i-\vec{x}_j|)|F_\alpha|^2\right)\\ &\geq \rho_{\alpha,\min}\int \left(|\nabla_i \Psi_\alpha^{(i)}|^2 + \tfrac12 \sum_{j\neq i} v(|\vec{x}_i-\vec{x}_j|)|\Psi_\alpha^{(i)}|^2\right).\end{aligned} \tag{5.30}$$

We now use Lemma 2.5 to get, for all $0 \leq \varepsilon \leq 1$,

$$(5.30) \geq \rho_{\alpha,\min}\int \left(\varepsilon|\nabla_i \Psi_\alpha^{(i)}|^2 + a(1-\varepsilon)U(t_i)|\Psi_\alpha^{(i)}|^2\right) \tag{5.31}$$

where t_i is the distance to the nearest neighbor of $\vec{x}_i$, c.f., (2.29), and U the potential (2.30).

Since $\Psi_\alpha = \phi^{\rm GP}(\vec{x}_i)\Psi_\alpha^{(i)}$ we can estimate

$$|\nabla_i\Psi_\alpha|^2 \leq 2\rho_{\alpha,\max}|\nabla_i\Psi_\alpha^{(i)}|^2 + 2|\Psi_\alpha^{(i)}|^2 N C_M \tag{5.32}$$

with

$$C_M = \frac{1}{N}\sup_{\vec{x}\in\Lambda_M}|\nabla\phi^{\rm GP}(\vec{x})|^2 = \sup_{\vec{x}\in\Lambda_M}|\nabla\phi^{\rm GP}_{1,Na}(\vec{x})|^2. \tag{5.33}$$

Since Na is fixed, C_M is independent of N. Inserting (5.32) into (5.31), summing over i and using $\rho^{\rm GP}(\vec{x}_i) \leq \rho_{\alpha,\max}$ in the last term of (5.25) (in the box α), we get

$$Q_\alpha(F_\alpha) \geq \frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} E^U_\varepsilon(n_\alpha, L) - 8\pi a\rho_{\alpha,\max}n_\alpha - \varepsilon C_M n_\alpha, \tag{5.34}$$

where L is the side length of the box and $E^U_\varepsilon(n_\alpha, L)$ is the ground state energy of

$$\sum_{i=1}^{n_\alpha}(-\tfrac{1}{2}\varepsilon\Delta_i + (1-\varepsilon)aU(t_i)) \tag{5.35}$$

in the box (c.f. (2.35)). We want to minimize (5.34) with respect to n_α and drop the subsidiary condition $\sum_\alpha n_\alpha = N$ in (5.27). This can only lower the minimum. For the time being we also ignore the last term in (5.34). (The total contribution of this term for all boxes is bounded by $\varepsilon C_M N$ and will be shown to be negligible compared to the other terms.)

Since the lower bound for the energy of Theorem 2.4 was obtained precisely from a lower bound to the operator (5.35), we can use the statement and proof of Theorem 2.4. From this we see that

$$E^U_\varepsilon(n_\alpha, L) \geq (1-\varepsilon)\frac{4\pi a n_\alpha^2}{L^3}(1 - CY_\alpha^{1/17}) \tag{5.36}$$

with $Y_\alpha = a^3 n_\alpha/L^3$, provided Y_α is small enough, $\varepsilon \geq Y_\alpha^{1/17}$ and $n_\alpha \geq (\mathrm{const.})Y_\alpha^{-1/17}$. The condition on ε is certainly fulfilled if we choose $\varepsilon = Y^{1/17}$ with $Y = a^3N/L^3$. We now want to show that the n_α minimizing the right side of (5.34) is large enough for (5.36) to apply.

If the minimum of the right side of (5.34) (without the last term) is taken for some $\bar{n}_\alpha$, we have

$$\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}}\left(E^U_\varepsilon(\bar{n}_\alpha+1, L) - E^U_\varepsilon(\bar{n}_\alpha, L)\right) \geq 8\pi a\rho_{\alpha,\max}. \tag{5.37}$$

On the other hand, we claim that

Lemma 5.3. *For any n*

$$E^U_\varepsilon(n+1, L) - E^U_\varepsilon(n, L) \leq 8\pi a\frac{n}{L^3}. \tag{5.38}$$

Proof. Denote the operator (5.35) by $\tilde{H}_n$, with $n_\alpha = n$, and let $\tilde{\Psi}_n$ be its ground state. Let t'_i be the distance to the nearest neighbor of $\vec{x}_i$ among the $n+1$ points $\vec{x}_1, \ldots, \vec{x}_{n+1}$ (without $\vec{x}_i$) and t_i the corresponding distance excluding $\vec{x}_{n+1}$. Obviously, for $1 \leq i \leq n$,

$$U(t'_i) \leq U(t_i) + U(|\vec{x}_i - \vec{x}_{n+1}|) \tag{5.39}$$

and

$$U(t'_{n+1}) \leq \sum_{i=1}^{n} U(|\vec{x}_i - \vec{x}_{n+1}|). \tag{5.40}$$

Therefore

$$\tilde{H}_{n+1} \leq \tilde{H}_n - \tfrac{1}{2}\varepsilon\Delta_{n+1} + 2a\sum_{i=1}^{n} U(|\vec{x}_i - \vec{x}_{n+1}|). \tag{5.41}$$

Using $\tilde{\Psi}_n/L^{3/2}$ as trial function for $\tilde{H}_{n+1}$ we arrive at (5.38). ∎

Eq. (5.38) together with (5.37) shows that $\bar{n}_\alpha$ is at least $\sim \rho_{\alpha,\max}L^3$. We shall choose $L \sim N^{-1/10}$, so the conditions needed for (5.36) are fulfilled for N large enough, since $\rho_{\alpha,\max} \sim N$ and hence $\bar{n}_\alpha \sim N^{7/10}$ and $Y_\alpha \sim N^{-2}$.

In order to obtain a lower bound on Q_α we therefore have to minimize

$$4\pi a \left(\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \frac{n_\alpha^2}{L^3} \left(1 - CY^{1/17}\right) - 2n_\alpha \rho_{\alpha,\max} \right). \tag{5.42}$$

We can drop the requirement that n_α has to be an integer. The minimum of (5.42) is obtained for

$$n_\alpha = \frac{\rho_{\alpha,\max}^2}{\rho_{\alpha,\min}} \frac{L^3}{(1 - CY^{1/17})}. \tag{5.43}$$

By Eq. (5.24) this gives the following lower bound, including now the last term in (5.34) as well as the contributions from the boxes outside Λ_M,

$$\begin{aligned} &E_0(N,a) - E^{\rm GP}(N,a) \geq \\ &4\pi a \int |\rho^{\rm GP}|^2 - 4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha,\min}^2 L^3 \left(\frac{\rho_{\alpha,\max}^3}{\rho_{\alpha,\min}^3} \frac{1}{(1 - CY^{1/17})} \right) \\ &- Y^{1/17} N C_M - 4\pi a N \sup_{\vec{x} \notin \Lambda_M} \rho^{\rm GP}(\vec{x}). \end{aligned} \tag{5.44}$$

Now $\rho^{\rm GP}$ is differentiable and strictly positive. Since all the boxes are in the fixed cube Λ_M there are constants $C' < \infty$, $C'' > 0$, such that

$$\rho_{\alpha,\max} - \rho_{\alpha,\min} \leq NC'L, \quad \rho_{\alpha,\min} \geq NC''. \tag{5.45}$$

Since $L \sim N^{-1/10}$ and $Y \sim N^{-17/10}$ we therefore have, for large N,

$$\frac{\rho_{\alpha,\max}^3}{\rho_{\alpha,\min}^3} \frac{1}{(1 - CY^{1/17})} \leq 1 + (\text{const.}) N^{-1/10} \tag{5.46}$$

Also,

$$4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha,\min}^2 L^3 \leq 4\pi a \int |\rho^{\rm GP}|^2 \leq E^{\rm GP}(N,a). \tag{5.47}$$

Hence, noting that $E^{\rm GP}(N,a) = NE^{\rm GP}(1,Na) \sim N$ since Na is fixed,

$$\frac{E_0(N,a)}{E^{\rm GP}(N,a)} \geq 1 - (\text{const.})(1 + C_M)N^{-1/10} - (\text{const.}) \sup_{\vec{x} \notin \Lambda_M} |\phi_{1,Na}^{\rm GP}|^2, \tag{5.48}$$

where the constants depend on Na. We can now take $N \to \infty$ and then $M \to \infty$.

Part 3: Lower bound to the QM energy, TF case. In the above proof of the lower bound in the GP case we did not attempt to keep track of the dependence of the constants on Na. In the TF case $Na \to \infty$, so one would need to take a closer look at this dependence if one wanted to carry the proof directly over to this case. But we don't have to do so, because there is a simpler direct proof. Using the explicit form of the TF minimizer, namely

$$\rho^{\mathrm{TF}}_{N,a}(\vec{x}) = \frac{1}{8\pi a}[\mu^{\mathrm{TF}} - V(\vec{x})]_+, \tag{5.49}$$

where $[t]_+ \equiv \max\{t, 0\}$ and μ^{TF} is chosen so that the normalization condition $\int \rho^{\mathrm{TF}}_{N,a} = N$ holds, we can use

$$V(\vec{x}) \geq \mu^{\mathrm{TF}} - 8\pi a \rho^{\mathrm{TF}}(\vec{x}) \tag{5.50}$$

to get a replacement as in (5.26), but without changing the measure. Moreover, ρ^{TF} has compact support, so, applying again the box method described above, the boxes far out do not contribute to the energy. However, μ^{TF} (which depends only on the combination Na) tends to infinity as $Na \to \infty$. We need to control the asymptotic behavior of μ^{TF}, and this leads to the restrictions on V described in the paragraph preceding Theorem 5.2. For simplicity, we shall here only consider the case when V itself is homogeneous, i.e., $V(\lambda\vec{x}) = \lambda^s V(\vec{x})$ for all $\lambda > 0$ with some $s > 0$.

In the same way as in (5.6) we have, with $g = Na$,

$$\mu^{\mathrm{TF}}(g) = dE^{\mathrm{TF}}(N,a)/dN = E^{\mathrm{TF}}(1,g) + 4\pi g \int |\rho^{\mathrm{TF}}_{1,g}(\vec{x})|^2 d\vec{x}. \tag{5.51}$$

The TF energy, chemical potential and minimizer satisfy the scaling relations

$$E^{\mathrm{TF}}(1,g) = g^{s/(s+3)} E^{\mathrm{TF}}(1,1), \tag{5.52}$$

$$\mu^{\mathrm{TF}}(g) = g^{s/(s+3)} \mu^{\mathrm{TF}}(1), \tag{5.53}$$

and

$$g^{3/(s+3)} \rho^{\mathrm{TF}}_{1,g}(g^{1/(s+3)}\vec{x}) = \rho^{\mathrm{TF}}_{1,g}(\vec{x}). \tag{5.54}$$

We also introduce the scaled interaction potential, $\widehat{v}$, by

$$\widehat{v}(\vec{x}) = g^{2/(s+3)} v(g^{1/(s+3)}\vec{x}) \tag{5.55}$$

with scattering length

$$\widehat{a} = g^{-1/(s+3)} a. \tag{5.56}$$

Using (5.50), (5.51) and the scaling relations we obtain

$$E_0(N,a) \geq E^{\mathrm{TF}}(N,a) + 4\pi N g^{s/(s+3)} \int |\rho^{\mathrm{TF}}_{1,1}|^2 + g^{-2/(s+3)} Q \tag{5.57}$$

with

$$Q = \inf_{\int |\Psi|^2 = 1} \sum_i \int \left(|\nabla_i \Psi|^2 + \tfrac{1}{2} \sum_{j \neq i} \widehat{v}(\vec{x}_i - \vec{x}_j)|\Psi|^2 - 8\pi N \widehat{a} \rho^{\mathrm{TF}}_{1,1}(\vec{x}_i)|\Psi|^2 \right). \tag{5.58}$$

We can now proceed exactly as in Part 2 to arrive at the the analogy of Eq. (5.44), which in the present case becomes

$$E_0(N,a) - E^{\mathrm{TF}}(N,a) \geq \\ 4\pi N g^{s/(s+3)} \int |\rho^{\mathrm{TF}}_{1,1}|^2 - 4\pi N \widehat{a} \sum_\alpha \rho^2_{\alpha,\max} L^3 (1 - C\widehat{Y}^{1/17})^{-1}. \tag{5.59}$$

Here $\rho_{\alpha,\max}$ is the maximum of $\rho^{\mathrm{TF}}_{1,1}$ in the box α, and $\widehat{Y} = \widehat{a}^3 N/L^3$. This holds as long as L does not decrease too fast with N. In particular, if L is simply fixed, this holds for all large enough N. Note that

$$\bar{\rho} = N\bar{\rho}_{1,g} \sim N g^{-3/(s+3)} \bar{\rho}_{1,1}, \tag{5.60}$$

so that $\widehat{a}^3 N \sim a^3 \bar{\rho}$ goes to zero as $N \to \infty$ by assumption. Hence, if we first let $N \to \infty$ (which implies $\widehat{Y} \to 0$) and then take L to zero, we of arrive at the desired result

$$\liminf_{N\to\infty} \frac{E_0(N,a)}{E^{\mathrm{TF}}(N,a)} \geq 1 \tag{5.61}$$

in the limit $N \to \infty$, $a^3\bar{\rho} \to 0$. Here we used the fact that (because V, and hence ρ^{TF}, is continuous by assumption) the Riemann sum $\sum_\alpha \rho^2_{\alpha,\max} L^3$ converges to $\int |\rho^{\mathrm{TF}}_{1,1}|^2$ as $L \to 0$. Together with the upper bound (5.22) and the fact that $E^{\mathrm{GP}}(N,a)/E^{\mathrm{TF}}(N,a) = E^{\mathrm{GP}}(1,Na)/E^{\mathrm{TF}}(1,Na) \to 1$ as $Na \to \infty$, which holds under our regularity assumption on V (c.f. Lemma 2.3 in [LSeY2]), this proves (5.14) and (5.17).

Part 4: Convergence of the densities. The convergence of the energies implies the convergence of the densities in the usual way by variation of the external potential. We show here the TF case, the GP case goes analogously. Set again $g = Na$. Making the replacement

$$V(\vec{x}) \longrightarrow V(\vec{x}) + \delta g^{s/(s+3)} Z(g^{-1/(s+3)}\vec{x}) \tag{5.62}$$

for some positive $Z \in C_0^\infty$ and redoing the upper and lower bounds we see that (5.17) holds with W replaced by $W + \delta Z$. Differentiating with respect to δ at $\delta = 0$ yields

$$\lim_{N\to\infty} \frac{g^{3/(s+3)}}{N} \rho^{\mathrm{QM}}_{N,a}(g^{1/(s+3)}\vec{x}) = \tilde{\rho}^{\mathrm{TF}}_{1,1}(\vec{x}) \tag{5.63}$$

in the sense of distributions. Since the functions all have L^1-norm 1, we can conclude that there is even weak L^1-convergence. ■

5.2. **Two Dimensions.** In contrast to the three-dimensional case the energy per particle for a dilute gas in two dimensions is *nonlinear* in ρ. In view of Schick's formula (3.1) for the energy of the homogeneous gas it would appear natural to take the interaction into account in two dimensional GP theory by a term

$$4\pi \int_{\mathbb{R}^2} |\ln(|\phi(\vec{x})|^2 a^2)|^{-1} |\phi(\vec{x})|^4 d\vec{x}, \tag{5.64}$$

and such a term has, indeed, been suggested in [Sh] and [KNSQ]. However, since the nonlinearity appears only in a logarithm, this term is unnecessarily complicated as far as leading order computations are concerned. For dilute gases it turns out to be sufficient, to leading order, to use an interaction term of the same form as in the three-dimensional case, i.e, define the GP functional as (for simplicity we put $\mu = 1$ in this section)

$$\mathcal{E}^{\rm GP}[\phi] = \int_{\mathbb{R}^2} \left(|\nabla\phi|^2 + V|\phi|^2 + 4\pi\alpha|\phi|^4 \right) d\vec{x}, \tag{5.65}$$

where instead of a the coupling constant is now

$$\alpha = |\ln(\bar{\rho}_N a^2)|^{-1} \tag{5.66}$$

with $\bar{\rho}_N$ the *mean density* for the GP functional at coupling constant 1 and particle number N. This is defined analogously to (5.12) as

$$\bar{\rho}_N = \frac{1}{N} \int |\phi^{\rm GP}_{N,1}|^4 d\vec{x} \tag{5.67}$$

where $\phi^{\rm GP}_{N,1}$ is the minimizer of (5.65) with $\alpha = 1$ and subsidiary condition $\int |\phi|^2 = N$. Note that α in (5.66) depends on N through the mean density.

Let us denote the GP energy for a given N and coupling constant α by $E^{\rm GP}(N,\alpha)$ and the corresponding minimizer by $\phi^{\rm GP}_{N,\alpha}$. As in three dimensions the scaling relations

$$E^{\rm GP}(N,\alpha) = NE^{\rm GP}(1, N\alpha) \tag{5.68}$$

and

$$N^{-1/2}\phi^{\rm GP}_{N,\alpha} = \phi^{\rm GP}_{1,N\alpha}, \tag{5.69}$$

hold, and the relevant parameter is

$$g \equiv N\alpha. \tag{5.70}$$

In three dimensions, where $\alpha = a$, it is natural to consider the limit $N \to \infty$ with $g = Na=$ const. The analogue of Theorem 5.1 in two dimensions is

Theorem 5.4 (Two-dimensional GP limit theorem). *If, for $N \to \infty$, $a^2\bar{\rho}_N \to 0$ with $g = N/|\ln(a^2\bar{\rho}_N)|$ fixed, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\rm GP}(N, 1/|\ln(a^2\bar{\rho}_N)|)} = 1 \tag{5.71}$$

and

$$\lim_{N\to\infty} \frac{1}{N}\rho^{\rm QM}_{N,a}(\vec{x}) = \left|\phi^{\rm GP}_{1,g}(\vec{x})\right|^2 \tag{5.72}$$

in the weak L^1-sense.

This result, however, is of rather limited use in practice. The reason is that in two dimensions the scattering length has to decrease exponentially with N if g is fixed. The parameter g is typically *very large* in two dimensions so it is more appropriate to consider the limit $N \to \infty$ and $g \to \infty$ (but still $\bar{\rho}_N a^2 \to 0$).

For potentials V that are *homogeneous* functions of $\vec{x}$, i.e.,

$$V(\lambda \vec{x}) = \lambda^s V(\vec{x}) \tag{5.73}$$

for some $s > 0$, this limit can be described by the a 'Thomas-Fermi' energy functional like (5.16) with coupling constant unity:

$$\mathcal{E}^{\rm TF}[\rho] = \int_{\mathbb{R}^2} \left(V(\vec{x})\rho(\vec{x}) + 4\pi\rho(\vec{x})^2 \right) d\vec{x}. \tag{5.74}$$

This is just the GP functional without the gradient term and $\alpha = 1$. Here ρ is a nonnegative function on $\mathbb{R}^2$ and the normalization condition is

$$\int \rho(\vec{x}) d\vec{x} = 1. \tag{5.75}$$

The minimizer of (5.74) can be given explicitly. It is

$$\rho^{\rm TF}_{1,1}(\vec{x}) = (8\pi)^{-1}[\mu^{\rm TF} - V(\vec{x})]_+ \tag{5.76}$$

where the chemical potential $\mu^{\rm TF}$ is determined by the normalization condition (5.75) and $[t]_+ = t$ for $t \geq 0$ and zero otherwise. We denote the corresponding energy by $E^{\rm TF}(1,1)$. By scaling one obtains

$$\lim_{g\to\infty} E^{\rm GP}(1,g)/g^{s/(s+2)} = E^{\rm TF}(1,1), \tag{5.77}$$

$$\lim_{g\to\infty} g^{2/(s+2)} \rho^{\rm GP}_{1,g}(g^{1/(s+2)}\vec{x}) = \rho^{\rm TF}_{1,1}(\vec{x}), \tag{5.78}$$

with the latter limit in the strong L^2 sense.

Our main result about two-dimensional Bose gases in external potentials satisfying (5.73) is that analogous limits also hold for the many-particle quantum mechanical ground state at low densities:

Theorem 5.5 (Two-dimensional TF limit theorem). *In two dimensions, if $a^2\bar{\rho}_N \to 0$, but $g = N/|\ln(\bar{\rho}_N a^2)| \to \infty$ as $N \to \infty$ then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{g^{s/s+2}} = E^{\rm TF}(1,1) \tag{5.79}$$

and, in the weak L^1 sense,

$$\lim_{N\to\infty} \frac{g^{2/(s+2)}}{N} \rho^{\rm QM}_{N,a}(g^{1/(s+2)}\vec{x}) = \rho^{\rm TF}_{1,1}(\vec{x}). \tag{5.80}$$

Remarks: 1. As in Theorem 5.2, it is sufficient that V is asymptotically equal to some homogeneous potential, W. In this case, $E^{\rm TF}(1,1)$ and $\rho^{\rm TF}_{1,1}$ in Theorem 5.5 should be replaced by the corresponding quantities for W.

2. From Eq. (5.78) it follows that

$$\bar{\rho}_N \sim N^{s/(s+2)} \tag{5.81}$$

for large N. Hence the low density criterion $a^2\bar{\rho} \ll 1$, means that $a/L_{\rm osc} \ll N^{-s/2(s+2)}$.

We shall now comment briefly on the proofs of Theorems 5.4 and 5.5, mainly pointing out the differences from the 3D case considered previously.

The upper bounds for the energy are obtained exactly in a same way as in three dimensions. For the lower bound in Theorem 5.4 the point to notice is that the expression (5.42), that has to be minimized over n_α, is in 2D replaced by

$$4\pi\left(\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}}\frac{n_\alpha^2}{L^2}\frac{1}{|\ln(a^2n_\alpha/L^2)|}\left(1-\frac{C}{|\ln(a^2N/L^2)|^{1/5}}\right)-\frac{2n_\alpha\rho_{\alpha,\max}}{|\ln(a^2\bar{\rho}_N)|}\right), \tag{5.82}$$

since Eq. (5.36) has to be replaced by the analogous inequality for 2D (c.f. (3.31)). To minimize (5.82) we use the following lemma:

Lemma 5.6. *For $0<x,b<1$ and $k\geq 1$ we have*

$$\frac{x^2}{|\ln x|}-2\frac{b}{|\ln b|}xk \geq -\frac{b^2}{|\ln b|}\left(1+\frac{1}{(2|\ln b|)^2}\right)k^2. \tag{5.83}$$

Proof. Replacing x by x/k and using the monotonicity of ln we see that it suffices to consider $k=1$. Since $\ln x \geq -\frac{1}{de}x^{-d}$ for all $d>0$ we have

$$\frac{x^2}{b^2}\frac{|\ln b|}{|\ln x|}-2\frac{x}{b} \geq \frac{|\ln b|}{b^2}edx^{2+d}-\frac{2x}{b} \geq c(d)(b^d ed|\ln b|)^{-1/(1+d)} \tag{5.84}$$

with

$$c(d)=2^{(2+d)/(1+d)}\left(\frac{1}{(2+d)^{(2+d)/(1+d)}}-\frac{1}{(2+d)^{1/(1+d)}}\right)\geq -1-\frac{1}{4}d^2. \tag{5.85}$$

Choosing $d=1/|\ln b|$ gives the desired result. ■

Applying this lemma with $x=a^2n_\alpha/L^2$, $b=a^2\rho_{\alpha,\max}$ and

$$k=\frac{\rho_{\alpha,\max}}{\rho_{\alpha,\min}}\left(1-\frac{C}{|\ln(a^2N/L^2)|^{1/5}}\right)^{-1}\frac{|\ln(a^2\rho_{\alpha,\max})|}{|\ln(a^2\bar{\rho}_N)|} \tag{5.86}$$

we get the bound

$$(5.82) \geq -4\pi\frac{\rho_{\alpha,\max}^2L^2}{|\ln(a^2\bar{\rho}_N)|}\left(1+\frac{1}{4|\ln(a^2\rho_{\alpha,\max})|^2}\right)k. \tag{5.87}$$

In the limit considered, k and the factor in parenthesis both tend to 1 and the Riemann sum over the boxes α converges to the integral as $L\to 0$.

The TF case, Thm. 5.5, is treated in the same way as in three dimensions, with modifications analogous to those just discussed when passing from 3D to 2D in GP theory.

6. BEC for Dilute Trapped Gases

It is gratifying to see the experimental realization, in traps, of the long-predicted Bose-Einstein condensation (BEC) of gases. From the theoretical point of view, however, a rigorous demonstration of this phenomenon – starting from the many-body Hamiltonian of interacting particles – has not yet been achieved. Following [LSe], we will provide in this section such a rigorous justification for the ground state of 2D or 3D bosons in a trap with repulsive pair potentials, and in the well-defined limit in which the Gross-Pitaevskii (GP) formula is applicable. It is the first proof of BEC for interacting particles in a continuum (as distinct from lattice) model and in a physically realistic situation. The Gross-Pitaevskii limit under discussion here is, of course, a physically simpler limit than the usual thermodynamic limit in which the average density is held fixed as the particle number goes to infinity. In the GP limit one also lets the range of the potential go to zero as N goes to infinity, but in such a way that the overall effect is non-trivial. That is, the combined effect of the infinite particle limit and the zero range limit is such as to leave a measurable residue — the GP function.

It was shown in the previous section (see also Theorem 6.3 below) that, for each fixed Na, the minimization of the GP functional correctly reproduces the large N asymptotics of the ground state energy and density of H – but no assertion about BEC in this limit was made. We will now extend this result by showing that in the Gross-Pitaevskii limit there is indeed 100% Bose condensation in the ground state. This is a generalization of the homogeneous case considered in Theorem 4.1. In the following, we concentrate on the 3D case, but analogous considerations apply also to the 2D case.

For use later, we define the projector

$$P^{\mathrm{GP}} = |\varphi^{\mathrm{GP}}\rangle\langle\varphi^{\mathrm{GP}}| \ . \tag{6.1}$$

Here (and everywhere else in this section) we denote $\varphi^{\mathrm{GP}} = \phi^{\mathrm{GP}}_{1,Na}$ for simplicity, where $\phi^{\mathrm{GP}}_{1,Na}$ is the minimizer of the GP functional (5.2) with parameter Na and normalization condition $\int|\phi|^2 = 1$ (compare with (5.8)). Moreover, we set $\mu \equiv 1$.

In the following, Ψ_0 denotes the (nonnegative and normalized) ground state of the Hamiltonian (5.1). BEC refers to the reduced one-particle density matrix $\gamma(\vec{x},\vec{x}')$ of Ψ_0, defined in (4.1).

Complete (or 100%) BEC is defined to be the property that $\frac{1}{N}\gamma(\vec{x},\vec{x}')$ not only has an eigenvalue of order one, as in the general case of an incomplete BEC, but in the limit it has only one nonzero eigenvalue (namely 1). Thus, $\frac{1}{N}\gamma(\vec{x},\vec{x}')$ becomes a simple product $\varphi(\vec{x})^*\varphi(\vec{x}')$ as $N\to\infty$, in which case φ is called the *condensate wave function*. In the GP limit, i.e., $N\to\infty$ with Na fixed, we can show that this is the case, and the condensate wave function is, in fact, the GP minimizer φ^{GP}.

Theorem 6.1 (**Bose-Einstein condensation**). *For each fixed Na*

$$\lim_{N\to\infty}\frac{1}{N}\gamma(\vec{x},\vec{x}')=\varphi^{\rm GP}(\vec{x})\varphi^{\rm GP}(\vec{x}')\ .$$

in trace norm, i.e., $\mathrm{Tr}\left|\frac{1}{N}\gamma-P^{\rm GP}\right|\to 0$.

We remark that Theorem 6.1 implies that there is also 100% condensation for all n-particle reduced density matrices

$$\begin{aligned}&\gamma^{(n)}(\vec{x}_1,\ldots,\vec{x}_n;\vec{x}_1',\ldots,\vec{x}_n')\\&=n!\binom{N}{n}\int\Psi_0(\vec{x}_1,\ldots,\vec{x}_N)\Psi_0(\vec{x}_1',\ldots,\vec{x}_n',\vec{x}_{n+1},\ldots\vec{x}_N)d\vec{x}_{n+1}\cdots d\vec{x}_N\end{aligned}\tag{6.2}$$

of Ψ_0, i.e., they converge, after division by the normalization factor, to the one-dimensional projector onto the n-fold tensor product of $\varphi^{\rm GP}$. In other words, for n fixed particles the probability of finding them all in the same state $\varphi^{\rm GP}$ tends to 1 in the limit considered. To see this, let a^*,a denote the boson creation and annihilation operators for the state $\varphi^{\rm GP}$, and observe that

$$1\geq\lim_{N\to\infty}N^{-n}\langle\Psi_0|(a^*)^na^n|\Psi_0\rangle=\lim_{N\to\infty}N^{-n}\langle\Psi_0|(a^*a)^n|\Psi_0\rangle\ ,\tag{6.3}$$

since the terms coming from the commutators $[a,a^*]=1$ are of lower order as $N\to\infty$ and vanish in the limit. From convexity it follows that

$$N^{-n}\langle\Psi_0|(a^*a)^n|\Psi_0\rangle\geq N^{-n}\langle\Psi_0|a^*a|\Psi_0\rangle^n\tag{6.4}$$

which converges to 1 as $N\to\infty$, proving our claim.

Another corollary, important for the interpretation of experiments, concerns the momentum distribution of the ground state.

Corollary 6.2 (**Convergence of momentum distribution**). *Let*

$$\widehat{\rho}(\vec{k})=\int\int\gamma(\vec{x},\vec{x}')\exp[i\vec{k}\cdot(\vec{x}-\vec{x}')]d\vec{x}d\vec{x}'$$

denote the one-particle momentum density of Ψ_0. Then, for fixed Na,

$$\lim_{N\to\infty}\frac{1}{N}\widehat{\rho}(\vec{k})=|\widehat{\varphi}^{\rm GP}(\vec{k})|^2$$

strongly in $L^1(\mathbb{R}^3)$. Here, $\widehat{\varphi}^{\rm GP}$ denotes the Fourier transform of $\varphi^{\rm GP}$.

Proof. If $\mathcal{F}$ denotes the (unitary) operator 'Fourier transform' and if h is an arbitrary L^∞-function, then

$$\begin{aligned}\left|\frac{1}{N}\int\widehat{\rho}h-\int|\widehat{\varphi}^{\rm GP}|^2h\right|&=\left|\mathrm{Tr}\,[\mathcal{F}^{-1}(\gamma/N-P^{\rm GP})\mathcal{F}h]\right|\\&\leq\|h\|_\infty\mathrm{Tr}\,|\gamma/N-P^{\rm GP}|,\end{aligned}$$

from which we conclude that

$$\|\widehat{\rho}/N-|\widehat{\varphi}^{\rm GP}|^2\|_1\leq\mathrm{Tr}\,|\gamma/N-P^{\rm GP}|\ .$$

∎

Before proving Theorem 6.1, let us state some prior results on which we shall build. Then we shall formulate two lemmas, which will allow us to prove Theorem 6.1.

The following theorem is an extension of Theorem 5.1.

Theorem 6.3 (Asymptotics of the energy components). *If ψ_0 denotes the solution to the zero-energy scattering equation for v (under the boundary condition $\lim_{|\vec{x}|\to\infty}\psi_0(\vec{x})=1$) and $s=\int|\nabla\psi_0|^2/(4\pi a)$, then $0<s\leq 1$ and*

$$\lim_{N\to\infty}\int|\nabla_{\vec{x}_1}\Psi_0(\vec{x}_1,\vec{X})|^2 d\vec{x}_1\,d\vec{X}$$

$$=\int|\nabla\varphi^{\mathrm{GP}}(\vec{x})|^2 d\vec{x}+4\pi Nas\int|\varphi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x}, \tag{6.5a}$$

$$\lim_{N\to\infty}\int V(\vec{x}_1)|\Psi_0(\vec{x}_1,\vec{X})|^2 d\vec{x}_1\,d\vec{X}=\int V(\vec{x})|\varphi^{\mathrm{GP}}(\vec{x})|^2 d\vec{x}, \tag{6.5b}$$

$$\lim_{N\to\infty}\tfrac{1}{2}\sum_{j=2}^{N}\int v(|\vec{x}_1-\vec{x}_j|)|\Psi_0(\vec{x}_1,\vec{X})|^2 d\vec{x}_1\,d\vec{X}$$

$$=(1-s)4\pi Na\int|\varphi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x}. \tag{6.5c}$$

Here we introduced again the short hand notation

$$\vec{X}=(\vec{x}_2,\dots,\vec{x}_N)\qquad\text{and}\quad d\vec{X}=\prod_{j=2}^{N}d\vec{x}_j. \tag{6.6}$$

Theorem 6.3 is a simple consequence of Theorem 5.1 by variation with respect to the different components, in the same way as was explained in the proof of Theorem 4.1, c.f. Eqs. (4.7)–(4.9). This was also noted in [CS2].

As already stated, Theorem 6.1 is a generalization of Theorem 4.1, the latter corresponding to the case that V is a box potential. It should be noted, however, that we use different scaling conventions in these two theorems: In Theorem 4.1 the box size grows as $N^{1/3}$ to keep the density fixed, while in Theorem 6.1 we choose to keep the confining external potential fixed. Both conventions are equivalent, of course, c.f. the remark at the end of Section 4, but when comparing the exponents of N that appear in the proofs of the two theorems the different conventions should be born in mind.

There are two essential components of our proof of Theorem 6.1. The first is a proof that the part of the kinetic energy that is associated with the interaction v (namely, the second term in (6.5a)) is mostly located in small balls surrounding each particle. More precisely, these balls can be taken to have radius roughly $N^{-5/9}$, which is much smaller than the mean-particle spacing $N^{-1/3}$. This allows us to conclude that the function of $\vec{x}$ defined for each fixed value of $\vec{X}$ by

$$f_{\vec{X}}(\vec{x})=\frac{1}{\varphi^{\mathrm{GP}}(\vec{x})}\Psi_0(\vec{x},\vec{X})\geq 0 \tag{6.7}$$

has the property that $\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})$ is almost zero outside the small balls centered at points of $\vec{X}$.

The complement of the small balls has a large volume but it can be a weird set; it need not even be connected. Therefore, the smallness of $\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})$ in this set does not guarantee that $f_{\vec{X}}(\vec{x})$ is nearly constant (in $\vec{x}$), or even that it is continuous. We need $f_{\vec{X}}(\vec{x})$ to be nearly constant in order to conclude BEC. What saves the day is the knowledge that the total kinetic energy of $f_{\vec{X}}(\vec{x})$ (including the balls) is not huge. The result that allows us to combine these two pieces of information in order to deduce the almost constancy of $f_{\vec{X}}(\vec{x})$ is the generalized Poincaré inequality in Lemma 6.5.

Using the results of Theorem 6.3, partial integration and the GP equation (i.e., the variational equation for φ^{GP}, see Eq. (5.5)) we see that

$$\lim_{N\to\infty} \int |\varphi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 d\vec{x}\, d\vec{X} = 4\pi N a s \int |\varphi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x} \ . \tag{6.8}$$

The following Lemma shows that to leading order all the energy in (6.8) is concentrated in small balls.

Lemma 6.4 (**Localization of the energy**). *For fixed $\vec{X}$ let*

$$\Omega_{\vec{X}} = \left\{ \vec{x} \in \mathbb{R}^3 \ \middle| \ \min_{k\geq 2} |\vec{x} - \vec{x}_k| \geq N^{-1/3-\delta} \right\} \tag{6.9}$$

for some $0 < \delta < 2/9$. Then

$$\lim_{N\to\infty} \int d\vec{X} \int_{\Omega_{\vec{X}}} d\vec{x} |\varphi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 = 0 \ .$$

Remark. In the proof of Theorem 4.1 we chose δ to be $4/51$, but the following proof shows that one can extend the range of δ beyond this value.

Proof. We shall show that

$$\begin{aligned}
&\int d\vec{X} \int_{\Omega^c_{\vec{X}}} d\vec{x}\, |\varphi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 \\
&+\tfrac{1}{2} \int d\vec{X} \int d\vec{x}\, |\varphi^{\mathrm{GP}}(\vec{x})|^2 \sum_{k\geq 2} v(|\vec{x} - \vec{x}_k|) |f_{\vec{X}}(\vec{x})|^2 \\
&-8\pi N a \int d\vec{X} \int d\vec{x}\, |\varphi^{\mathrm{GP}}(\vec{x})|^4 |f_{\vec{X}}(\vec{x})|^2 \\
&\geq -4\pi N a \int |\varphi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x} - o(1)
\end{aligned} \tag{6.10}$$

as $N \to \infty$, which implies the assertion of the Lemma by virtue of (6.8) and the results of Theorem 6.3. Here, $\Omega^c_{\vec{X}}$ is the complement of $\Omega_{\vec{X}}$. The proof of (6.10) is actually just a detailed examination of the lower bounds to the energy derived in [LSeY1] and [LY1] and described in Sections 2 and 5. We use the same methods as there, just describing the differences from the case considered here.

Writing

$$f_{\vec{X}}(\vec{x}) = \prod_{k\geq 2} \varphi^{\rm GP}(\vec{x}_k) F(\vec{x}, \vec{X}) \tag{6.11}$$

and using that F is symmetric in the particle coordinates, we see that (6.10) is equivalent to

$$\frac{1}{N} Q_\delta(F) \geq -4\pi N a \int |\varphi^{\rm GP}|^4 - o(1), \tag{6.12}$$

where Q_δ is the quadratic form

$$\begin{aligned} Q_\delta(F) &= \sum_{i=1}^N \int_{\Omega_i^c} |\nabla_i F|^2 \prod_{k=1}^N |\varphi^{\rm GP}(\vec{x}_k)|^2 d\vec{x}_k \\ &\quad + \sum_{1\leq i<j\leq N} \int v(|\vec{x}_i - \vec{x}_j|)|F|^2 \prod_{k=1}^N |\varphi^{\rm GP}(\vec{x}_k)|^2 d\vec{x}_k \\ &\quad -8\pi N a \sum_{i=1}^N \int |\varphi^{\rm GP}(\vec{x}_i)|^2 |F|^2 \prod_{k=1}^N |\varphi^{\rm GP}(\vec{x}_k)|^2 d\vec{x}_k. \end{aligned} \tag{6.13}$$

Here Ω_i^c denotes the set

$$\Omega_i^c = \{(\vec{x}_1, \vec{X}) \in \mathbb{R}^{3N} \,|\, \min_{k\neq i} |\vec{x}_i - \vec{x}_k| \leq N^{-1/3-\delta}\}.$$

While (6.12) is not true for all conceivable F's satisfying the normalization condition

$$\int |F(\vec{x}, \vec{X})|^2 \prod_{k=1}^N |\varphi^{\rm GP}(\vec{x}_k)|^2 d\vec{x}_k = 1,$$

it *is* true for an F, such as ours, that has bounded kinetic energy (6.8). Looking at Section 5, we see that Eqs. (5.24)–(5.25), (5.44)–(5.48) are similar to (6.12), (6.13) and almost establish (6.12), but there are differences which we now explain.

In our case, the kinetic energy of particle i is restricted to the subset of $\mathbb{R}^{3N}$ in which $\min_{k\neq i} |\vec{x}_i - \vec{x}_k| \leq N^{-1/3-\delta}$. However, looking at the proof of the lower bound to the ground state energy of a homogeneous Bose gas discussed in Section 2, which enters the proof of Theorem 5.1, we see that if we choose $\delta \leq 4/51$ only this part of the kinetic energy is needed for the lower bound, except for some part with a relative magnitude of the order $\varepsilon = O(N^{-2\alpha})$ with $\alpha = 1/17$. (Here we use the a priori knowledge that the kinetic energy is bounded by (6.8). See also the analogous discussion in Section 4, p. 23.) We can even do better and choose some $4/51 < \delta < 2/9$, if α is chosen small enough. (To be precise, we choose $\beta = 1/3 + \alpha$ and $\gamma = 1/3 - 4\alpha$ in the notation of (2.56), and α small enough). The choice of α only affects the magnitude of the error term, however, which is still $o(1)$ as $N \to \infty$.

Proceeding exactly as in Section 5 and taking the differences just mentioned into account we arrive at (6.12). ■

In the following, $\mathcal{K} \subset \mathbb{R}^m$ denotes a bounded and connected set that is sufficiently nice so that the Poincaré-Sobolev inequality (see [LLo], Thm. 8.12) holds on $\mathcal{K}$. In particular, this is the case if $\mathcal{K}$ satisfies the cone property [LLo] (e.g., if $\mathcal{K}$ is a ball or a cube). The next Lemma generalizes Lemma 4.2.

Lemma 6.5 (**Generalized Poincaré inequality**). *For $d \geq 2$ let $\mathcal{K} \subset \mathbb{R}^d$ be as explained above, and let h be a bounded function with $\int_{\mathcal{K}} h = 1$. There exists a constant C (depending only on $\mathcal{K}$ and h) such that for all measurable sets $\Omega \subset \mathcal{K}$ and all $f \in H^1(\mathcal{K})$ with $\int_{\mathcal{K}} f h \, d\vec{x} = 0$, the inequality*

$$\int_{\mathcal{K}} |f(\vec{x})|^2 d\vec{x} \leq C \left(\int_{\Omega} |\nabla f(\vec{x})|^2 d\vec{x} + \left(\frac{|\Omega^c|}{|\mathcal{K}|} \right)^{2/d} \int_{\mathcal{K}} |\nabla f(\vec{x})|^2 d\vec{x} \right) \tag{6.14}$$

holds. Here $|\cdot|$ denotes the measure of a set, and $\Omega^c = \mathcal{K} \setminus \Omega$.

Proof. By the usual Poincaré-Sobolev inequality on $\mathcal{K}$ (see [LLo], Thm. 8.12),

$$\begin{aligned} \|f\|^2_{L^2(\mathcal{K})} &\leq \tilde{C} \|\nabla f\|^2_{L^{2d/(d+2)}(\mathcal{K})} \\ &\leq 2\tilde{C} \left(\|\nabla f\|^2_{L^{2d/(d+2)}(\Omega)} + \|\nabla f\|^2_{L^{2d/(d+2)}(\Omega^c)} \right), \end{aligned} \tag{6.15}$$

if $d \geq 2$ and $\int_{\mathcal{K}} fh = 0$. Applying Hölder's inequality

$$\|\nabla f\|_{L^{2d/(d+2)}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} |\Omega|^{1/d}$$

(and the analogue with Ω replaced by Ω^c), we see that (6.14) holds with $C = 2|\mathcal{K}|^{2/d} \tilde{C}$. ■

The important point in Lemma 6.5 is that there is no restriction on Ω concerning regularity or connectivity.

Proof of Theorem 6.1. For some $R > 0$ let $\mathcal{K} = \{\vec{x} \in \mathbb{R}^3, |\vec{x}| \leq R\}$, and define

$$\langle f_{\vec{X}} \rangle_{\mathcal{K}} = \frac{1}{\int_{\mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 d\vec{x}} \int_{\mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 f_{\vec{X}}(\vec{x}) \, d\vec{x} \, .$$

We shall use Lemma 6.5, with $d = 3$, $h(\vec{x}) = |\varphi^{\rm GP}(\vec{x})|^2 / \int_{\mathcal{K}} |\varphi^{\rm GP}|^2$, $\Omega = \Omega_{\vec{X}} \cap \mathcal{K}$ and $f(\vec{x}) = f_{\vec{X}}(\vec{x}) - \langle f_{\vec{X}} \rangle_{\mathcal{K}}$ (see (6.9) and (6.7)). Since $\varphi^{\rm GP}$ is bounded on $\mathcal{K}$ above and below by some positive constants, this Lemma also holds (with a different constant C') with $d\vec{x}$ replaced by $|\varphi^{\rm GP}(\vec{x})|^2 d\vec{x}$ in

(6.14). Therefore,

$$\int d\vec{X} \int_{\mathcal{K}} d\vec{x} |\varphi^{\rm GP}(\vec{x})|^2 \left[f_{\vec{X}}(\vec{x}) - \langle f_{\vec{X}} \rangle_{\mathcal{K}} \right]^2$$
$$\leq C' \int d\vec{X} \left[\int_{\Omega_{\vec{X}} \cap \mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 d\vec{x} + \frac{N^{-2\delta}}{R^2} \int_{\mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 d\vec{x} \right], \tag{6.16}$$

where we used that $|\Omega^c_{\vec{X}} \cap \mathcal{K}| \leq (4\pi/3) N^{-3\delta}$. The first integral on the right side of (6.16) tends to zero as $N \to \infty$ by Lemma 6.4, and the second is bounded by (6.8). We conclude, since

$$\int_{\mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 f_{\vec{X}}(\vec{x}) d\vec{x} \leq \int_{\mathbb{R}^3} |\varphi^{\rm GP}(\vec{x})|^2 f_{\vec{X}}(\vec{x}) d\vec{x}$$

because of the positivity of $f_{\vec{X}}$, that

$$\begin{aligned} \liminf_{N\to\infty} \frac{1}{N} \langle \varphi^{\rm GP} | \gamma | \varphi^{\rm GP} \rangle &\geq \int_{\mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 d\vec{x} \lim_{N\to\infty} \int d\vec{X} \int_{\mathcal{K}} d\vec{x} |\Psi_0(\vec{x}, \vec{X})|^2 \\ &= \left[\int_{\mathcal{K}} |\varphi^{\rm GP}(\vec{x})|^2 d\vec{x} \right]^2, \end{aligned}$$

where the last equality follows from (5.15). Since the radius of $\mathcal{K}$ was arbitrary, we conclude that

$$\lim_{N\to\infty} \frac{1}{N} \langle \varphi^{\rm GP} | \gamma | \varphi^{\rm GP} \rangle = 1,$$

implying convergence of γ/N to $P^{\rm GP}$ in Hilbert-Schmidt norm. Since the traces are equal, convergence even holds in trace norm (cf. [Si], Thm. 2.20), and Theorem 6.1 is proven. ■

We remark that the method presented here also works in the case of a two-dimensional Bose gas. The relevant parameter to be kept fixed in the GP limit is $N/|\ln(a^2\bar{\rho}_N)|$, all other considerations carry over without essential change, using the results in [LSeY2, LY2], c.f. Sections 3 and 5.2. A minor difference concerns the parameter s in Theorem 6.3, which can be shown to be always equal to 1 in 2D, i.e., the interaction energy is purely kinetic in the GP limit (see [CS1]). It should be noted that the existence of BEC in the ground state in 2D is not in conflict with its absence at positive temperatures [Ho, M]. In the hard core lattice gas at half filling precisely this phenomenon occurs [KLS]. We also point out that our method necessarily fails for the one-dimensional Bose gas, where there is presumably no BEC [PiSt]. An analogue of Lemma 6.4 cannot hold in the 1D case since even a hard core potential with arbitrarily small range produces an interaction energy that is not localized on scales smaller than the mean particle spacing.

7. The Charged Bose Gas

The setting now changes abruptly. Instead of particles interacting with a short-range potential $v(|\vec{x}_i - \vec{x}_j|)$ they interact via the Coulomb potential

$$v(|\vec{x}_i - \vec{x}_j|) = |\vec{x}_i - \vec{x}_j|^{-1}$$

(in 3 dimensions). There are N particles in a large box Λ of volume L^3 as before, with $\rho = N/L^3$.

To offset the huge Coulomb repulsion (which would drive the particles to the walls of the box) we add a uniform negative background of precisely the same charge, namely density ρ. Our Hamiltonian is thus

$$H = \sum_{i=1}^{N} -\mu\Delta_i - V(\vec{x}_i) + \sum_{1\leq i<j\leq N} v(|\vec{x}_i - \vec{x}_j|) + C \tag{7.1}$$

with

$$V(\vec{x}) = \rho \int_\Lambda |\vec{x} - \vec{y}|^{-1} d\vec{y} \qquad \text{and} \qquad C = \frac{1}{2}\rho \int_\Lambda V(\vec{x}) d\vec{x}\ .$$

Each particle interacts only with others and not with itself. Thus, despite the fact that the Coulomb potential is positive definite, the ground state energy E_0 can be (and is) negative (just take Ψ =const.). This time, *large* ρ is the 'weakly interacting' regime.

We know from the work in [LN] that the thermodynamic limit $e_0(\rho)$ defined as in (2.2) exists.

Another way in which this problem is different from the previous one is that *perturbation theory is correct to leading order.* If one computes $(\Psi, H\Psi)$ with Ψ =const, one gets the right first order answer, namely 0. It is the next order in $1/\rho$ that is interesting, and this is *entirely* due to correlations. In 1961 Foldy [F] calculated this correlation energy according to the prescription of Bogolubov's 1947 theory. That theory was not exact for the dilute Bose gas, as we have seen, even to first order. We are now looking at *second* order, which should be even worse. Nevertheless, there was good physical intuition that this calculation should be asymptotically *exact.* Indeed it is, as proved in [LSo].

The Bogolubov theory states that the main contribution to the energy comes from pairing of particles into momenta $\vec{k}, -\vec{k}$ and is the bosonic analogue of the BCS theory of superconductivity which came a decade later. I.e., Ψ_0 is a sum of products of terms of the form $\exp\{i\vec{k}\cdot(\vec{x}_i - \vec{x}_j)\}$.

Foldy's energy, based on Bogolubov's ansatz, has now been proved. His calculation essentially implies an upper bound as proved by Dyson in [D2] for a slight reformulation of the model. The lower bound is the hard part.

Theorem 7.1 (Foldy's law).

$$\lim_{\rho\to\infty} \rho^{-1/4} e_0(\rho) \geq -\frac{2}{5}\frac{\Gamma(3/4)}{\Gamma(5/4)}\left(\frac{2}{\mu\pi}\right)^{1/4} . \tag{7.2}$$

This is the *first example* (in more than 1 dimension) in which Bogolubov's pairing theory has been rigorously validated. It has to be emphasized, however, that Foldy and Bogolubov rely on the existence of Bose-Einstein condensation. We neither make such a hypothesis nor does our result for the energy imply the existence of such condensation. As we said earlier, it is sufficient to prove condensation in small boxes of fixed size.

Incidentally, the one-dimensional example for which Bogolubov's theory is asymptotically exact to the first two orders (high density) is the repulsive delta-function Bose gas [LL].

To appreciate the $-\rho^{1/4}$ nature of (7.2), it is useful to compare it with what one would get if the bosons had infinite mass, i.e., the first term in (7.1) is dropped. Then the energy would be proportional to $-\rho^{1/3}$ as shown in [LN]. Thus, the effect of quantum mechanics is to lower $\frac{1}{3}$ to $\frac{1}{4}$.

It is supposedly true that there is a critical mass above which the ground state should show crystalline ordering (Wigner crystal), but this has never been proved and it remains an intriguing open problem, even for the infinite mass case. A simple scaling shows that large mass is the same as small ρ, and is thus outside the region where a Bogolubov approximation can be expected to hold.

Another important remark about the $-\rho^{1/4}$ law is its relation to the $-N^{7/5}$ law for a *two*-component charged Bose gas. Dyson [D2] proved that the ground state energy for such a gas was at least as negative as $-(\text{const})N^{7/5}$ as $N \to \infty$. Thus, thermodynamic stability (i.e., a linear lower bound) fails for this gas. Years later, a lower bound of this $-N^{7/5}$ form was finally established in [CLY], thereby proving that this law is correct. The connection of this $-N^{7/5}$ law with the jellium $-\rho^{1/4}$ law (for which a corresponding lower bound was also given in [CLY]) was pointed out by Dyson [D2] in the following way. Assuming the correctness of the $-\rho^{1/4}$ law, one can treat the 2-component gas by treating each component as a background for the other. What should the density be? If the gas has a radius L and if it has N bosons then $\rho = NL^{-3}$. However, the extra kinetic energy needed to compress the gas to this radius is NL^{-2}. The total energy is then $NL^{-2} - N\rho^{1/4}$, and minimizing this with respect to L leads to the $-N^{7/5}$ law. A proof going in the other direction is in [CLY].

A problem somewhat related to bosonic jellium is *fermionic* jellium. Graf and Solovej [GS] have proved that the first two terms are what one would expect, namely

$$e_0(\rho) = C_{\text{TF}}\rho^{5/3} - C_{\text{D}}\rho^{4/3} + o(\rho^{4/3}), \tag{7.3}$$

where C_{TF} is the usual Thomas-Fermi constant and C_{D} is the usual Dirac exchange constant.

As for the dilute Bose gas there are several relevant length scales in the problem of the charged Bose gas. For the dilute gas there were three scales. This time there are just two. Because of the long range nature of the Coulomb problem there is no scale corresponding to the scattering length a.

One relevant length scale is again the interparticle distance $\rho^{-1/3}$. The other is the correlation length scale $\ell_{\rm cor} \sim \rho^{-1/4}$ (ignoring the dependence on μ). The order of the correlation length scale can be understood heuristically as follows. Localizing on a scale $\ell_{\rm cor}$ requires kinetic energy of the order of $\ell_{\rm cor}^{-2}$. The Coulomb potential from the particles and background on the scale $\ell_{\rm cor}$ is $(\rho\ell_{\rm cor}^3)/\ell_{\rm cor}$. Thus the kinetic energy and the Coulomb energy balance when $\ell_{\rm cor} \sim \rho^{-1/4}$. This heuristics is however much too simplified and hides the true complexity of the situation.

Note that in the high density limit $\ell_{\rm cor}$ is long compared to the interparticle distance. This is analogous to the dilute gas where the scale ℓ_c is also long compared to the interparticle distance [see (2.12)]. There is however no real analogy between the scale $\ell_{\rm cor}$ for the charged gas and the scale ℓ_c for the dilute gas. In particular, whereas $e_0(\rho)$ for the dilute gas is up to a constant of the same order as the kinetic energy $\sim \mu\ell_c^{-2}$ we have for the charged gas that $e_0(\rho) \not\sim \ell_{\rm cor}^{-2} = \rho^{1/2}$. The reason for this difference is that on average only a small fraction of the particles in the charged gas actually correlate.

7.1. **A Short Sketch of the Rigorous Proof.**

Step 1: Localization into small boxes: As mentioned above an important step in the rigorous proof is again to divide the big box Λ into smaller boxes of some fixed size ℓ. This time we must require $\ell_{\rm cor} \ll \ell$. We again use Neumann boundary conditions on the boundary of each little box.

In contrast to the dilute gas we can however no longer simply ignore the interaction between the small boxes. To overcome this problem we use a sliding technique first introduced in [CLY]. To explain this technique we introduce the localized interaction $w(\vec{x},\vec{y}) = \chi(\vec{x})Y_\omega(\vec{x}-\vec{y})\chi(\vec{y})$, where $Y_\omega(\vec{x}) = |\vec{x}|^{-1}\exp(-\omega|\vec{x}|)$ is a Yukawa potential and χ is a smooth approximation to the characteristic function of the cube $[0,\ell]^3$. Consider the Hamiltonian

$$H_\ell = \sum_{j=1}^{N}\left(-\mu\gamma^{-1}\Delta_{\ell,j} - \rho\int w(\vec{x}_j,\vec{y})\,d\vec{y}\right) + \sum_{1\le i<j\le N} w(\vec{x}_i,\vec{x}_j) + \tfrac{1}{2}\rho^2\iint w(\vec{x},\vec{y})\,d\vec{x}\,d\vec{y}, \tag{7.4}$$

where $-\Delta_\ell$ is the Neumann Laplacian for the cube $[0,\ell]^3$, and γ is a constant depending on χ that converges to 1 as χ converges to the characteristic function of $[0,\ell]^3$. We consider $-\Delta_\ell$ as acting in the Hilbert space $L^2(\mathbb{R}^3)$ in such a way that it is zero on functions supported away from $[0,\ell]^3$. Let $H_\ell(\vec{z})$ be the corresponding Hamiltonian for the translated box $\vec{z}+[0,\ell]^3$. If we ignore small errors (that can be fairly easily controlled) due to the boundary of Λ, the original operator H in (7.1) is bounded below by the operator

$$\ell^{-3}\gamma \int_\Lambda H_\ell(\vec{z})d\vec{z} - \frac{\omega N}{2\ell}. \tag{7.5}$$

The last error term is due to the interaction between the small boxes. This requires that the parameter ω is chosen appropriately. In fact, it must tend to infinity as χ converges to the characteristic function of $[0,\ell]^3$. If we make sure that $\ell \gg \omega\rho^{-1/4} = \omega\ell_{\rm cor}$ we have that $\omega N/\ell \ll N\rho^{1/4}$ and we may ignore this error term.

In the treatment of the dilute gas it was important to understand the distribution of particles into the different cells. This is not an issue here. In fact the presence of the background will imply that the smallest energy is achieved when the number of particles in each cell essentially neutralizes the background. More precisely we may simply look for a lower bound on the energy independent of the numbers of particles in each little box.

The operator H_ℓ was defined as an operator on $L^2(\mathbb{R}^{3N})$, but we may consider its restriction to the invariant subspace with precisely n particles in the box $[0,\ell]^3$. This restriction is equivalent to an operator H_ℓ^n acting on the space $L^2([0,\ell]^{3n})$. Note that H_ℓ^n has the form (7.4) with N replaced by n, except that now the Neumann Laplacian is considered as acting in $L^2([0,\ell]^3)$.

The problem of finding a lower bound on the ground state energy of H has been reduced to finding a lower bound on the operator H_ℓ^n independently of n for $0 \le n \le N$. Without discussing the proof of this point further we shall from now on use that it is essentially enough to consider $n = \rho\ell^3$ (the neutral case).

Step 2: Reducing to quadratic Hamiltonian: The next step is to use the second quantization formalism, which is the one used by Bogolubov and which is a very convenient bookkeeping device (but it has to be noted that it is no more than a convenient device and it does not introduce any new physics or mathematics). In second quantized form we may write the Hamiltonian H_ℓ^n as

$$\begin{aligned} H_\ell^n &= \mu\gamma^{-1}\sum_{\vec{p}} |\vec{p}|^2 a_{\vec{p}}^* a_{\vec{p}} + \tfrac{1}{2}\sum_{\vec{p}\vec{q},\vec{\mu}\vec{\nu}} \widehat{w}_{\vec{p}\vec{q},\vec{\mu}\vec{\nu}} a_{\vec{p}}^* a_{\vec{q}}^* a_{\vec{\nu}} a_{\vec{\mu}} - \rho\ell^3 \sum_{\vec{p}\vec{q}} \widehat{w}_{\vec{0}\vec{p},\vec{0}\vec{q}} a_{\vec{p}}^* a_{\vec{q}} \\ &\quad + \tfrac{1}{2}\rho^2\ell^6 \widehat{w}_{\vec{0}\vec{0},\vec{0}\vec{0}}, \end{aligned} \tag{7.6}$$

where $a_{\vec{p}}^*$ is the creation operator for the eigenfunction $u_{\vec{p}}$ of the Neumann Laplacian and

$$\widehat{w}_{\vec{p}\vec{q},\vec{\mu}\vec{\nu}} = \iint w(\vec{x},\vec{y}) u_{\vec{p}}(\vec{x}) u_{\vec{q}}(\vec{y}) u_{\vec{\mu}}(\vec{x}) u_{\vec{\nu}}(\vec{y})\, d\vec{x}\, d\vec{y}. \tag{7.7}$$

Through a very complicated bootstrapping procedure one now proves that to the order of interest here one may ignore several terms in H_ℓ^n and consider instead the Hamiltonian

$$\begin{aligned} H_{\mathrm{Q}} &= \mu\gamma^{-1}\sum_{\vec{p}}|\vec{p}|^2 a^*_{\vec{p}}a_{\vec{p}} \\ &\quad + \sum_{\vec{p}\vec{q}\neq\vec{0}} \widehat{w}_{\vec{p}\vec{q},\vec{0}\vec{0}}\left(a^*_{\vec{p}}a_{\vec{q}}a^*_{\vec{0}}a_{\vec{0}} + \tfrac{1}{2}a^*_{\vec{p}}a^*_{\vec{q}}a_{\vec{0}}a_{\vec{0}} + \tfrac{1}{2}a^*_{\vec{0}}a^*_{\vec{0}}a_{\vec{p}}a_{\vec{q}}\right). \end{aligned} \tag{7.8}$$

We have denoted this operator with a Q since it is quadratic in the operators $a^*_{\vec{p}}$, with $\vec{p}\neq\vec{0}$.

In order to reduce to this quadratic Hamiltonian it is important to be able to control the degree of condensation into the Neumann ground state, the constant function $u_{\vec{0}} = \ell^{-3/2}$. More precisely, if we denote by $\widehat{n}_+ = \sum_{\vec{p}\neq\vec{0}} a^*_{\vec{p}}a_{\vec{p}}$ the operator counting the number of particles not in the condensate, we would like to know that for the minimal energy state, the expectation $\langle\widehat{n}_+\rangle$ is small compared to the total particle number n. This, it turns out is not too difficult. One needs, however, also a good bound on $\langle\widehat{n}_+^2\rangle$ and this is more difficult. In [LSo] this is not achieved directly through a bound on $\langle\widehat{n}_+^2\rangle$ in the ground state. Rather it is proved that one may change the ground state without changing its energy very much, so that it only contains values of $\widehat{n}_+$ localized close to $\langle\widehat{n}_+\rangle$. This technique, which in [LSo] was called "localization of large matrices", allows one to consider only states where $\langle\widehat{n}_+^2\rangle \approx \langle\widehat{n}_+\rangle^2$.

Step 3: Controlling the kinetic energy: The final reduction of the Hamiltonian before one can apply the Bogolubov-Foldy method concerns the kinetic energy. In fact, if Δ denotes the Laplacian on $\mathbb{R}^3$ we shall use the bound (see Lemma 6.1 in [LSo])

$$\langle\phi, -\Delta_\ell\phi\rangle \geq \langle\phi, \chi_\ell F(-\Delta)\chi_\ell\phi\rangle\,, \text{ where } \quad F(v) = (1-Ct)\frac{v^2}{v+(\ell t^3)^{-2}}, \tag{7.9}$$

for functions ϕ orthogonal to constants and where we have assumed that the parameter t is chosen such that $\|\partial^\alpha\chi\|_\infty \leq t^{-|\alpha|}\ell^{-|\alpha|}$ for all multi-indices α with $|\alpha|\leq 3$. Here $C>0$ is some universal constant.

If we introduce the operator $b^*_{\vec{k}} = a^*(\chi_{\vec{k}})a_{\vec{0}}$, where $\chi_{\vec{k}}$ is the projection of the function $\chi(\vec{x})\exp(i\vec{k}\cdot\vec{x})$ onto the orthogonal complement of the constant functions, we can write the above inequality as

$$\sum_{\vec{p}}|\vec{p}|^2 a^*_{\vec{p}}a_{\vec{p}} \geq (2\pi)^{-3}n^{-1}\int F(|\vec{k}|^2)b^*_{\vec{k}}b_{\vec{k}}d\vec{k}. \tag{7.10}$$

Note the extra factor n^{-1} which is due to the fact that $b^*_{\vec{k}}$ contains a factor $a_{\vec{0}}$ and that we are considering states with total particle number n.

The reason that we have included a factor $a_{\vec{0}}$ in $b^*_{\vec{k}}$ is in order to be able to write the the last sum in H_Q also in terms of the $b^*_{\vec{k}}$. In fact, if we use that $w(\vec{x},\vec{y}) = \chi(\vec{x})Y_\omega(\vec{x}-\vec{y})w(\vec{y})$ we get that

$$H_{\rm Q} \geq \tfrac{1}{2}(2\pi)^{-3}\int_{\mathbb{R}^3} h(\vec{k})\,d\vec{k} - \sum_{\vec{p}\vec{q}\neq\vec{0}} \widehat{w}_{\vec{p}\vec{q},\vec{0}\vec{0}}a^*_{\vec{p}}a_{\vec{q}}, \tag{7.11}$$

where

$$\begin{aligned} h(\vec{k}) &= \mu\gamma^{-1}n^{-1}F(|\vec{k}|^2)\left(b^*_{\vec{k}}b_{\vec{k}} + b^*_{-\vec{k}}b_{-\vec{k}}\right) \\ &\quad + \widehat{Y}_\omega(\vec{k})\ell^{-3}\left(b^*_{\vec{k}}b_{\vec{k}} + b^*_{-\vec{k}}b_{-\vec{k}} + b^*_{\vec{k}}b^*_{-\vec{k}} + b_{\vec{k}}b_{-\vec{k}}\right). \end{aligned} \tag{7.12}$$

The last term in (7.11) comes from the fact that one must commute the factor $a_{\vec{0}}a^*_{\vec{0}}$ in $b^*_{\vec{k}}b_{\vec{k}}$ so that it occurs in the normal ordered way $a^*_{\vec{0}}a_{\vec{0}}$ as in H_Q. It is not difficult to see that one may ignore the last error term in (7.11) to the order of interest here.

Step 4. Applying Bogolubov's method: The last step in the analysis is now to use the following simple form of Bogolubov's method.

Theorem 7.2 (**Simple case of Bogolubov's method).**
For constants $\mathcal{A} \geq \mathcal{B} > 0$ and all $\vec{k}$ we have the operator inequality

$$\begin{aligned} &\mathcal{A}(b^*_{\vec{k}}b_{\vec{k}} + b^*_{-\vec{k}}b_{-\vec{k}}) + \mathcal{B}(b^*_{\vec{k}}b^*_{-\vec{k}} + b_{\vec{k}}b_{-\vec{k}}) \\ &\quad\geq\ -\tfrac{1}{2}(\mathcal{A} - \sqrt{\mathcal{A}^2-\mathcal{B}^2})([b_{\vec{k}}, b^*_{\vec{k}}] + [b_{-\vec{k}}, b^*_{-\vec{k}}]). \end{aligned}$$

Proof. We may complete the square

$$\begin{aligned} &\mathcal{A}(b^*_{\vec{k}}b_{\vec{k}} + b^*_{-\vec{k}}b_{-\vec{k}}) + \mathcal{B}(b^*_{\vec{k}}b^*_{-\vec{k}} + b_{\vec{k}}b_{-\vec{k}}) \\ &\quad=\ D(b^*_{\vec{k}} + \alpha b_{-\vec{k}})(b_{\vec{k}} + \alpha b^*_{-\vec{k}}) + D(b^*_{-\vec{k}} + \alpha b_{\vec{k}})(b_{-\vec{k}} + \alpha b^*_{-\vec{k}}) \\ &\quad\quad -D\alpha^2([b_{\vec{k}}, b^*_{\vec{k}}] + [b_{-\vec{k}}, b^*_{-\vec{k}}]), \end{aligned}$$

where

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

We choose the solution $\alpha = \mathcal{A}/\mathcal{B} - \sqrt{\mathcal{A}^2/\mathcal{B}^2 - 1}$. Hence

$$D\alpha^2 = \mathcal{B}\alpha/2 = \tfrac{1}{2}(\mathcal{A} - \sqrt{\mathcal{A}^2-\mathcal{B}^2}).$$

■

It is not difficult to see that $[b_{\vec{k}}, b^*_{\vec{k}}] \leq n\ell^3$. Using the theorem above we see that the ground state energy of H^n_ℓ up to the errors we have ignored is bounded below by $-\frac{1}{2}(2\pi)^{-3}\int f(\vec{k}) - (f(\vec{k})^2 - g(\vec{k})^2)^{1/2}d\vec{k}$, where $g(\vec{k}) = n\widehat{Y}_\omega(\vec{k})$ and $f(\vec{k}) = g(\vec{k}) + \mu\gamma^{-1}\ell^3F(|\vec{k}|^2)$.

Up to the order of interest we may now replace $\gamma^{-1}F(|\vec{k}|^2)$ by $|\vec{k}|^2$ and Y_ω by the Coulomb potential and thus $\widehat{Y}_\omega(\vec{k})$ by $4\pi|\vec{k}|^{-2}$. If we now also replace n by $\rho\ell^3$ we see that the ground state energy of H^n_ℓ to leading order is given by

$$-\tfrac{1}{2}(2\pi)^{-3}\rho\ell^3\int (4\pi|\vec{k}|^{-2}+\rho^{-1}\mu|\vec{k}|^2-((4\pi|\vec{k}|^{-2}+\rho^{-1}\mu|\vec{k}|^2)^2-(4\pi|\vec{k}|^{-2})^2)^{1/2}d\vec{k}$$

$$= 2^{-1/2}\pi^{-3/4}\rho\ell^3(\rho/\mu)^{1/4}\int_0^\infty 1 + x^4 - x^2(2+x^4)^{1/2}dx.$$

If we finally use that the integral above is

$$\frac{2^{3/4}\sqrt{\pi}\Gamma(3/4)}{5\Gamma(5/4)}$$

and that the leading order of the ground state energy of the original operator H according to (7.5) is L^3/ℓ^3 times the ground state energy of H_ℓ^n (again ignoring γ) we arrive at Foldy's law (7.2).

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