THE BOSE GAS: A SUBTLE MANY-BODY PROBLEM

Elliott H. Lieb

ABSTRACT. Now that the properties of the ground state 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. One of these is that the leading term in the energy/particle is $4\pi a\rho$ where a is the scattering length of the 2-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 jointly with J. Yngvason 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. Another problem of great interest is the existence of Bose-Einstein condensation, and what little is known about this rigorously will also be discussed. 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 (with Yngvason and Seiringer) that the Gross-Pitaevskii equation correctly describes the ground state in the 'traps' actually used in the experiments. The other is a very recent proof (with Solovej) that Foldy's 1961 theory of a high density gas of charged particles correctly describes its ground state energy.

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 $\Psi(x_1, ..., x_N)$ is automatically symmetric in the coordinates $x_j \in R^3$ of the N particles, we are dealing necessarily with *'bosons'*. If we imposed the Pauli exclusion principle (antisymmetry) instead, apppropriate 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.

1991 *Mathematics Subject Classification.* 81V70, 35Q55, 46N50.

Supported in part by NSF Grant PHY-98 20650 A01.

©2000 by the author. Reproduction of this article, in its entirety, by any means, is permitted for non-commercial purposes.

For the proceedings of the *XIII International Congress of Mathematical Physics*, London, July 18-24, 2000.

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 three main topics.

1. The dilute, repulsive Bose gas at low density (2D and 3D) (with Jakob Yngvason).

2. Repulsive bosons in a trap (as used in recent experiments) and the 'Gross-Pitaevskii equation (with Robert Seiringer and Jakob Yngvason).

3. Foldy's 'jellium' model of charged particles in a neutralizing background (with Jan Philip Solovej)

The discussion below of topic 1 is taken from [**1**] (in 3-dimensions) and [**2**] (in 2-dimensions). That for topic 2 is taken from [**3**] (in 3-dimensions) and [**4**] (in 2-dimensions). Topic 3 is from [**5**]. See also [**6, 7**].

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 [**6**]. In terms of technical complexity, however, the third topic is the most involved and can be treated here only very briefly.

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 $v(|\vec{x}_i - \vec{x}_j|)$:

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

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

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

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 [**3**]. 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 Schroedinger equation

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

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

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

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 scattering equation,

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

with $u_0(0) = 0$. (The factor 2 in (2.6) comes from the reduced mass of the two particle problem.)

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 $e_0(\rho)$.

The genesis of an understanding of $e_0(\rho)$ was the pioneering work [**11**] of Bogolubov, and in the 50's and early 60's several derivations of (2.8) were presented [**12**], [**13**], even including higher order terms:

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

These early developments are reviewed in [**14**]. 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 [**15**]:

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

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 prsents 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

$$\ell_c = (\rho a)^{-1/2}.$$

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 sdistance 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)

$$a \ll \rho^{-1/3} \ll \ell_c$$

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 [**16**]. 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 u_0 the scattering solution and $f_0(r) = u_0(r)/r$, partial integration gives

$$\begin{aligned} \int_{|\vec{x}|\leq R} \{2\mu|\nabla f_0|^2 + v|f_0|^2\} d\vec{x} &= 4\pi \int_0^R \{2\mu[u_0'(r) - (u_0(r)/r)]^2 + v(r)|u_0(r)]^2\} dr \\ &= 8\pi\mu a |u_0(R)|^2/R^2 \to 8\pi\mu a \quad \text{for } R \to \infty, \end{aligned} \tag{2.11}$$

if u_0 is normalized so that $f_0(R) \to 1$ as $R \to \infty$. Moreover, for positive interaction potentials the scattering solution minimizes the quadratic form in (2.11) for each R with $u_0(0) = 0$ and $u_0(R)$ fixed as boundary conditions. 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 [**11**] presupposes the existence of Bose-Einstein condensation. Nevertheless, it is correct (for the energy) for the one-dimensional delta-function Bose gas [**17**], despite the fact that there is (presumably) no condensation in that case. 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 [**15**].

2.1. UPPER BOUND. The following generalization of Dyson's upper bound holds [**3**], [**10**]:

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*

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \frac{a}{b} + \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1-\frac{a}{b}\right)^8}. \tag{2.12}$$

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*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \leq \frac{1 - Y^{1/3} + Y^{2/3} - \frac{1}{2}Y}{(1-Y^{1/3})^8}. \tag{2.13}$$

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

Remark. The bound (2.12) 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

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

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 [**15**] we choose a trial function of the following form

$$\Psi(x_1,\dots,x_N) = F_1(x_1)\cdot F_2(x_1,x_2)\cdots F_N(x_1,\dots,x_N). \tag{2.15}$$

More specifically, $F_1 \equiv 1$ and F_i depends only on the distance of x_i to its nearest neighbor among the the points $x_1,\dots,x_{i-1}$ (taking the periodic boundary into account):

$$F_i(x_1,\dots,x_i) = f(t_i), \quad t_i = \min\left(|x_i - x_j|, j = 1,\dots,i-1\right), \tag{2.16}$$

with a function f satisfying

$$0 \le f \le 1, \quad f' \ge 0. \tag{2.17}$$

The intuition behind the ansatz (2.15) 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 (2.16) is computationally easier to handle than an ansatz of the type $\prod_{i<j} f(|x_i - x_j|)$, which might appear more natural in view of the heuristic remarks at the end of the last subection.

The function f is chosen to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \le r \le b, \\ 1 & \text{for } r > b, \end{cases} \tag{2.18}$$

with $f_0(r) = u_0(r)/r$. The estimates (2.12) and (2.14) are obtained by somewhat lengthy computations similar as in [**15**], but making use of (2.11). For details we refer to [**3**] and [**10**].

A test wave function with Dirichlet boundary condition may be obtained by localizing the wave function (2.15) on the length scale L. The energy cost per particle for this is $(\text{const.})/L^2$. □

2.2. LOWER BOUND. In the beginning it was explained why the lower bound for the bosonic ground state energy of (2.1) is not easy to obtain. The three different length scales 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*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \ge (1 - C\,Y^{1/17}) \tag{2.19}$$

with C a constant. If v does not have finite range, but decreases at least as fast as $1/r^{3+\varepsilon}$ at infinity with some $\varepsilon > 0$, then an analogous bound to (2.19) holds, but with C replaced by another constant and 1/17 by another exponent, both of which may depend on ε.

It should be noted right away that the error term $-C\,Y^{1/17}$ in (2.19) 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 [**10**].

As mentioned in the Introduction 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 (2.19) 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 the ground state energy of (2.1) with Neumann conditions satisfies*

$$E_0(N, L)/N \geq 4\pi\mu\rho a \left(1 - C\,Y^{1/17}\right) \tag{2.20}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are 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 other constants and another exponent for Y, holds also for potentials v of infinite range decreasing faster than $1/r^3$ 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 $\mathcal{B} \subset \mathbf{R}^3$ be star shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then for all differentiable functions ψ*

$$\int_{\mathcal{B}} \left[\mu|\nabla\psi|^2 + \tfrac{1}{2}v|\psi|^2\right] \geq \mu a \int_{\mathcal{B}} U|\psi|^2. \tag{2.21}$$

Proof. Actually, (2.21) holds with $\mu|\nabla\phi(\vec{x})|^2$ replaced by the (smaller) radial kinetic energy, $\mu|\partial\phi(\vec{x})/\partial r|^2$, and it suffices to prove the analog of (2.21) for the integral along each radial line with fixed angular variables. Along such a line we write $\phi(\vec{x}) = u(r)/r$ 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.,

$$U(r) = \frac{1}{R^2}\delta(r - R). \tag{2.22}$$

For such U the analog of (2.21) along the radial line is

(2.23)

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

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 (2.23) 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,

(2.24)
$$\int_0^R \{\mu[u_0'(r) - (u_0(r)/r)]^2 + \tfrac{1}{2}v(r)|u_0(r)]^2\}dr = \mu a|R-a|/R \geq \mu a|R-a|^2/R^2.$$

But $|R-a|^2/R^2$ is precisely the right side of (2.23) if u satisfies the normalization condition.

This derivation of (2.21) for the special case (2.22) 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 [**15**].

COROLLARY 2.6. For any U as in Lemma 2.5

$$H_N \geq \mu a W \tag{2.25}$$

with

$$W(\vec{x}_1, \ldots, \vec{x}_N) = \sum_{i=1}^N U(t_i), \tag{2.26}$$

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.,

$$t_i(\vec{x}_1, \ldots, \vec{x}_N) = \min_{j,\, j\neq i} |\vec{x}_i - \vec{x}_j|. \tag{2.27}$$

(Note that t_i has here a slightly different meaning than in (2.16), where it denoted the distance to the nearest neighbor among the $\vec{x}_j$ with $j \leq i-1$.)

Dyson considers in [**15**] a one parameter family of U's that is essentially the same as the following choice, which is convenient for the present purpose:

$$U_R(r) = \begin{cases} 3(R^3 - R_0^3)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise.} \end{cases} \tag{2.28}$$

We denote the corresponding interaction (2.26) by W_R. For the hard core gas one obtains

$$E(N,L) \geq \sup_R \inf_{(\vec{x}_1,\ldots,\vec{x}_N)} \mu a W_R(\vec{x}_1, \ldots, \vec{x}_N) \tag{2.29}$$

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

$$\inf_{(\vec{x}_1,\ldots,\vec{x}_N)} W_R(\vec{x}_1, \ldots, \vec{x}_N) \geq \left(\frac{A}{R^3} - \frac{B}{\rho R^6}\right) \tag{2.30}$$

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

$$E(N,L)/N \geq \frac{1}{10\sqrt{2}} 4\pi\mu\rho a. \tag{2.31}$$

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 (2.29) is zero because $U(r) = 0$ for $r < R_0$.

For these reasons we take another route. We still use Lemma 2.21 to get into the soft potential regime, but we do *not* sacrifice *all* the kinetic energy as in (2.25). Instead we write, for $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1-\varepsilon)H_N \geq \varepsilon T_N + (1-\varepsilon)H_N \tag{2.32}$$

with $T_N = -\sum_i \Delta_i$ and use (2.25) only for the part $(1-\varepsilon)H_N$. This gives

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu a W_R. \tag{2.33}$$

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 [**1**], gives

$$\begin{aligned} 4\pi\rho\left(1-\tfrac{1}{N}\right) &\geq \langle W_R\rangle_0/N \\ &\geq 4\pi\rho\left(1-\tfrac{1}{N}\right)\left(1-\tfrac{2R}{L}\right)^3\left(1+4\pi\rho(1-\tfrac{1}{N})(R^3-R_0^3)/3)\right)^{-1}. \end{aligned} \tag{2.34}$$

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 first order result (2.34) looks 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 (2.34) 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* [**18**] for the expectations 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

$$(H - E_0)(H - E_1) \geq 0 \tag{2.35}$$

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

$$E_0 \geq \langle H\rangle_0 - \frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0} \tag{2.36}$$

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 (2.36) by $E_1^{(0)}$.

From (2.34) and (2.36) we get the estimate

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1-\mathcal{E}(\rho,L,R,\varepsilon)) \tag{2.37}$$

with

$$\begin{aligned} 1-\mathcal{E}(\rho,L,R,\varepsilon) &= (1-\varepsilon)\left(1-\tfrac{1}{\rho L^3}\right)\left(1-\tfrac{2R}{L}\right)^3\left(1+\tfrac{4\pi}{3}\rho(1-\tfrac{1}{N})(R^3-R_0^3)\right)\Big)^{-1} \\ &\times \left(1-\frac{\mu a\big(\langle W_R^2\rangle_0-\langle W_R\rangle_0^2\big)}{\langle W_R\rangle_0\big(E_1^{(0)}-\mu a\langle W_R\rangle_0\big)}\right). \end{aligned} \tag{2.38}$$

To evaluate this further one may use the estimates (2.34) and the bound

$$\langle W_R^2\rangle_0 \leq 3\frac{N}{R^3-R_0^3}\langle W_R\rangle_0 \tag{2.39}$$

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 (2.38) is, up to unimportant constants and lower order terms, $\sim(\varepsilon L^{-2}-a\rho^2L^3)$. 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 (2.38), 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. This boundary condition leads to lower energy than any other boundary condition. 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

$$E_0(N,L)/N \geq (\rho\ell^3)^{-1}\inf\sum_{n\geq 0} c_n E_0(n,\ell) \tag{2.40}$$

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

$$\sum_{n\geq 0} c_n = 1, \qquad \sum_{n\geq 0} c_n n = \rho\ell^3. \tag{2.41}$$

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

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1-\mathcal{E}(\rho,\ell,R,\varepsilon)) \tag{2.42}$$

i.e., replacement of L in (2.37) 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

$$E_0(n+n',\ell) \geq E_0(n,\ell) + E_0(n',\ell) \tag{2.43}$$

which follows immediately from $v \geq 0$ by dropping the interactions between the n particles and the n' particles. The bound (2.43) implies in particular that for any $n, p \in \mathbb{N}$ with $n \geq p$

$$E(n,\ell) \geq [n/p]\, E(p,\ell) \geq \frac{n}{2p} E(p,\ell) \tag{2.44}$$

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

The way (2.44) is used is as follows: Replacing L by ℓ, N by n and ρ by n/ℓ^3 in (2.37) we have for fixed R and ε

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1) K(n,\ell) \tag{2.45}$$

with a certain function $K(n,\ell)$ determined by (2.38). We shall see that K is monotonously decreasing in n, so that if $p \in \mathbb{N}$ and $n \leq p$ then

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1) K(p,\ell). \tag{2.46}$$

We now split the sum in (2.40) into two parts. For $n < p$ we use (2.46), and for $n \geq p$ we use (2.44) together with (2.46) for $n = p$. The task is thus to minimize

$$\sum_{n<p} c_n n(n-1) + \tfrac{1}{2} \sum_{n \geq p} c_n n(p-1) \tag{2.47}$$

subject to the constraints (2.41). Putting

$$k := \rho\ell^3 \quad \text{and} \quad t := \sum_{n<p} c_n n \leq k \tag{2.48}$$

we have $\sum_{n\geq p} c_n n = k - t$, and since $n(n-1)$ is convex in n, and $\sum_{n<p} c_n \leq 1$ the expression (2.47) is

$$\geq t(t-1) + \tfrac{1}{2}(k-t)(p-1). \tag{2.49}$$

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

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho \left(1 - \frac{1}{\rho\ell^3}\right) K(4\rho\ell^3, \ell). \tag{2.50}$$

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 (2.38) and (2.39) we obtain

$$\begin{aligned} K(n,\ell) &= (1-\varepsilon)\left(1 - \tfrac{2R}{\ell}\right)^3 \left(1 + \tfrac{4\pi}{3}\rho(1-\tfrac{1}{n})(R^3 - R_0^3)\right)^{-1} \\ &\times \left(1 - \frac{3}{\pi} \frac{an}{(R^3 - R_0^3)(\varepsilon\ell^{-2} - 4a\ell^{-3}n(n-1))}\right). \end{aligned} \tag{2.51}$$

The estimate (2.45) with this K is valid as long as the denominator in the last factor in (2.51) 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 (2.45) is negative. As required for (2.46), K is monotonously decreasing in n. We now insert $n = 4\rho\ell^3$ and obtain

$$\begin{aligned} K(4\rho\ell^3,\ell) &\geq (1-\varepsilon)\left(1-\tfrac{2R}{\ell}\right)^3 \left(1+(\text{const.})Y(\ell/a)^3(R^3-R_0^3)/\ell^3\right)^{-1} \\ &\times \left(1-\frac{\ell^3}{(R^3-R_0^3)}\frac{(\text{const.})Y}{(\varepsilon(a/\ell)^2-(\text{const.})Y^2(\ell/a)^3)}\right) \end{aligned} \tag{2.52}$$

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

$$\left(1-\frac{1}{\rho\ell^3}\right) = (1-(\text{const.})Y^{-1}(a/\ell)^3) \tag{2.53}$$

in (2.50) (which is the ratio between $n(n-1)$ and n^2) must not be be forgotten. We now make the ansatz

$$\varepsilon \sim Y^\alpha, \quad a/\ell \sim Y^\beta, \quad (R^3-R_0^3)/\ell^3 \sim Y^\gamma \tag{2.54}$$

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 (2.52).

Taking

$$\alpha = 1/17, \quad \beta = 6/17, \quad \gamma = 3/17 \tag{2.55}$$

all these conditions are satisfied, and

$$\alpha = 3\beta - 1 = 1 - 3\beta + \gamma = 1 - \alpha - 2\beta - \gamma = 1/17. \tag{2.56}$$

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 3.1 and 3.2, for the case of potentials with finite range. By optimizing the proportionality constants in (2.54) one can show that $C = 8.9$ is possible in Theorem 1.1 [**10**]. The extension to potentials of infinite range decreasing faster than $1/r^3$ at infinity is obtained by approximation by finite range potentials, controlling the change of the scattering length as the cut-off is removed. See Appendix B in [**3**] for details. A slower decrease than $1/r^3$ implies infinite scattering length. □

The exponents (2.55) mean in particular that

$$a \ll R \ll \rho^{-1/3} \ll \ell \ll (\rho a)^{-1/2}, \tag{2.57}$$

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

The two-dimensional theory, in contrast, began to receive attention only relatively late. The first derivation of the asymptotic formula was, to our knowledge, done by Schick [**19**], as late as 1971! He found

$$e_0(\rho) \simeq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}. \tag{3.1}$$

The scattering length a in (3.1) 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 [**2**].

Note that the answer could not possibly be $e_0(\rho) \simeq 4\pi\mu\rho a$ because that would be dimensionally wrong. But $e_0(\rho)$ must essentially be proportional to ρ, which leaves 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 $8\pi\mu L^{-2}\left[\ln(L^2/a^2)\right]^{-1}$. Thus, if the $N(N-1)/2$ rule were to apply in 2D, (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 it remains true 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 2D result is not a trivial extension of [**1**].

The proof of (3.1) is in [**2**]. The (relative) error terms to (3.1) givein in [**2**] are $|\ln(\rho a^2)|^{-1}$ for the upper bound and $|\ln(\rho a^2)|^{-1/5}$

To prove (3.1) the essential new step is to modify Dyson's lemma for 2D. The rest of the proof parallels that for 3D. The 2D version of Lemma 2.5 is [**2**]:

LEMMA 3.1. *Let $v(r) \geq 0$ with finite range R_0. Let $U(r) \geq 0$ be any function satisfying $\int U(r)\ln(r/a)rdr \leq 1$ and $U(r) = 0$ for $r < R_0$. Let $\mathcal{B} \subset \mathbf{R}^3$ be star shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then for all differentiable functions ψ*

$$\int_{\mathcal{B}} \left[\mu|\nabla\psi|^2 + \tfrac{1}{2}v|\psi|^2\right] \geq \mu\int_{\mathcal{B}} U|\psi|^2. \tag{3.2}$$

4. BOSE-EINSTEIN CONDENSATION

Let us comment very briefly 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 $L^2(\mathbf{R}^n)$ ($n = 2$ or 3) given by the kernel

$$\gamma(\vec{x}, \vec{y}) = N\int_{\mathrm{BOX}^{N-1}} \Psi_0(\vec{x}, \vec{x}_2, \ldots, \vec{x}_N)\Psi_0(\vec{y}, \vec{x}_2, \ldots, \vec{x}_N)d\vec{x}_2 \cdots d\vec{x}_N.$$

Then $\int \gamma(\vec{x}, \vec{x})d\vec{x} = \mathrm{Trace}(\gamma) = N$. BEC is the assertion that this operator has an eigenvalue of order N. 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 (volume)$^{-1/2}$. Therefore, another way to say that BEC exists is that

$$\int\int \gamma(\vec{x},\, \vec{y}) d\vec{x} d\vec{y} = \mathrm{O}(N).$$

Unfortunately, this is something that is frequently invoked but never proved — 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 [**20**].

The problem remains open after about 70 years. It is not at all clear that BEC is essential for superfluidity, as frequently claimed. Our construction in section 2 shows that BEC exists on a length scale of order $\rho^{-1/3}Y^{-1/17}$ which, unfortunately, is not a 'thermodynamic' length like volume$^{1/3}$.

5. GROSS-PITAEVSKII EQUATION FOR TRAPPED BOSONS

In the recent experiments on Bose condensation, the particles have to be confined in a cold 'trap' instead of a 'box' and we are certainly not at the 'thermodynamic limit'. For a 'trap' we add a *slowly* varying confining potential V, with $V(\vec{x}) \to \infty$ as $|\vec{x}| \to \infty$. The Hamiltonian becomes

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

If $v = 0$, then

$$\Psi_0(\vec{x}_1, \ldots, \vec{x}_N) = \textstyle\prod_{i=1}^{N} \Phi_0(\vec{x}_i)$$

with Φ_0= normalized ground state of $-\Delta + V(\vec{x})$ with eigenvalue $= \lambda$.

The idea is 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). This has been done with Robert Seiringer and Jakob Yngvason [**3, 4**].

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 GP energy functional

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

with the subsidiary condition

$$\int_{R^3} |\Phi|^2 = N$$

and corresponding energy

$$E^{\mathrm{GP}}(N,a) = \inf\{\mathcal{E}^{\mathrm{GP}}[\Phi] \;:\; \int |\Phi|^2 = N\} = \mathcal{E}^{\mathrm{GP}}[\Phi^{\mathrm{GP}}]. \tag{5.3}$$

As before, a is the scattering length of v.

It is not hard to prove that for every choice of the real number N there is a unique minimizer for Φ^{GP} for $\mathcal{E}^{\mathrm{GP}}$.

Relation of $\mathcal{E}^{\rm GP}$ and E_0: If $v = 0$ then clearly $\Phi^{\rm GP} = \sqrt{N}\ \Phi_0$, and then $\mathcal{E}^{\rm GP} = N\lambda = E_0$. 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 we take $\Phi^{\rm GP} \approx \sqrt{N/L^3}$ and we get $E^{\rm GP}(N) = 4\pi\mu a N^2/L^3$ = previous, homogeneous E_0 in the low density regime. (In this case, the gradient term in $\mathcal{E}^{\rm GP}[\Phi]$ plays no role.)

In general, we expect that $E^{\rm GP} = E_0$ in a suitable limit. This limit has to be chosen so that *all three* terms in $\mathcal{E}^{\rm GP}[\Phi]$ make a contribution. It turns out that fixing Na is the right thing to do (and this can be quite good experimentally since Na can range from about 1 to 1000).

THEOREM 5.1. *If $a_1 = Na$ is fixed,*

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

Moreover, the GP density is a limit of the QM density (convergence in weak L_1-sense):

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

We could imagine, instead, an $N \to \infty$ limit in which $a \gg N^{-1}$, i.e. $a_1 \to \infty$, but still $\bar{\rho}a^3 \to 0$, where $\bar{\rho}$ is the average density, given by

$$\bar{\rho} = \frac{1}{N}\int (\Phi^{\rm GP})^4. \tag{5.4}$$

In this case we simply omit the $\int |\nabla\Phi|^2$ term in $\mathcal{E}^{\rm GP}$; this theory is usually called 'Thomas-Fermi theory', but it has nothing to do with the fermionic theory invented by Thomas and Fermi in 1927. It is appropriate for the case in which Na is much bigger than 1, e.g., $Na \approx 1000$.

PROOF. Outline: Getting an upper bound for E_0 in terms of $E^{\rm GP}$ is relatively easy, as before. The problem is the lower bound.

One might suppose that one decomposes R^3 into small boxes as before, with Neumann b.c. on each box, and in each box one approximates $V(\vec{x})$ by a constant.

This will NOT work, even if $v = 0$, because all the particles will then want to be in the box with the smallest value of V. The gradient term will vanish and we will not get $E^{GP} = N\lambda$.

The trick is to write the quantum Ψ_0 as

$$\Psi_0 = \textstyle\prod_{i=1}^N \Phi^{\rm GP}(\vec{x}_i) F(\vec{x}_1, \ldots, \vec{x}_N).$$

This leads to a variational problem for F instead of Ψ_0. Partial integration and the variational equation for $\Phi^{\rm GP}$ lead to the replacements:

$$\text{External potential: } V(\vec{x}) \quad \to \quad -8\pi a|\Phi^{\rm GP}(\vec{x})|^2$$

and

$$\text{Measure: } \textstyle\prod_{i=1}^N d\vec{x}_i \quad \to \quad \prod_{i=1}^N |\Phi^{\rm GP}(\vec{x}_i)|^2 d\vec{x}_i.$$

We have to show that, with these replacements, the energy is bounded below by $-4\pi\mu a \int |\Phi^{\rm GP}|^4$ (up to small errors). *Now* we can effectively use the Neumann box method on *this* F problem.

There are still plenty of technical difficulties, but the back of the problem has been broken by recasting it in terms of F instead of Ψ_0. □

5.2. TWO-DIMENSIONS. In view of the two-dimensional result (3.1) we might suppose that we must replace $4\pi\mu a\Phi^4$ in (5.2) by $4\pi\mu\Phi^4/|\ln(\Phi^2a^2)|$, as suggested by (3.1). This is indeed correct, and a limit theorem for the energy and density is obtained that is similar to Theorem 5.1. There is a difference, however. This time one has to fix the ratio $N/\ln a$ instead of Na.

Since the logarithm is such a slowly varying function it turns out that one can still get the correct limit and yet simplify the problem by replacing $|\ln(\Phi^2a^2)|^{-1}$ in the functional by the constant $|\ln(\bar\rho a^2)|^{-1}$, where $\bar\rho$ is the average density in (5.4), but for 2D, of course.

6. 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 of volume L^3 as before, with $\rho = N/L^3$. We know from the work in [**21**] that a nice thermodynamic limit exists for $e_0 = E_0/N$.

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

$$H = -\mu\sum_{i=1}^{N}\Delta_i - V(\vec{x}_i) + \sum_{1\le i<j\le N} v(\vec{x}_i - \vec{x}_j) + C \tag{6.1}$$

with

$$V(\vec{x}) = \rho\int_{\rm BOX}|\vec{x}-\vec{y}|^{-1}d^3y \qquad \text{and} \qquad C = \frac{1}{2}\rho\int_{\rm BOX}V(\vec{x})d^3x\ .$$

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

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 [**22**] 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. It is!* and this was recently proved with Jan Philip Solovej [**5**].

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 germs of the form $\exp\{i\vec{k}\cdot(\vec{x}_i - \vec{x}_j)\}$.

Foldy's energy, based on Boglubov's ansatz, has now been proved. His calculation yields an upper bound. The lower bound is the hard part, and Solovej and I do this using the decomposition into 'Neumann boxes' as above. But unlike the short

range case, many complicated gymnastics are needed to control the long range $|\vec{x}|^{-1}$ Coulomb potential. The two bounds agree to leading order in ρ, namely $\rho^{1/4}$ (although there is an unimportant technical point that different boundary conditions are used for the two bounds).

THEOREM 6.1. *For large* ρ

$$e_0(\rho) \approx -0.402\, r_s^{-3/4} \frac{me^4}{\hbar^2} \tag{6.2}$$

where $r_s = (3/4\pi\rho)^{1/3} e^2 m/\hbar^2$.

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 [**17**]

To appreciate the $-\rho^{1/4}$ nature of (6.2), it is useful to compare it with what one would get if the bosons had infinite mass, i.e., the first term in (6.1) is dropped. Then the energy would be proportional to $-\rho^{1/3}$ as shown in [**21**]. 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. Since the relevant parameter is r_s, large mass is the same as small ρ, and is 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 [**23**] 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 [**24**], 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 [**24**]) was pointed out by Dyson [**23**] 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 [**24**].

A problem somewhat related to bosonic jellium is *fermionic* jellium. Graf and Solovej [**25**] have proved that the first two terms are what one would expect, namely

$$e(\rho) = C_{TF}\rho^{5/3} - C_D\rho^{4/3} + o(\rho^{4/3}),$$

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

Let us conclude with a few more details about some of the technicalities.

6.1. FOLDY'S CALCULATION, PAIRING THEORY AND IDEAS IN THE RIGOROUS PROOF. Foldy uses periodic boundary conditions for $-\Delta$, so the problem is on a torus. In order to make the Coulomb potential periodic and to take care of the background he replaces $|x-y|^{-1}$ by

$$\sum_{p\neq 0} L^{-3}|p|^{-2}\exp(ip(x-y)),$$

where the sum is over 'periodic momenta', p. (Note the $p\neq 0$ condition, so the spatial average of this potential is 0).

Foldy's Hamiltonian is

$$H' = \sum_{i=1}^{N} -\tfrac{1}{2}\Delta_i + \sum_{i<j}\sum_{p\neq 0} L^{-3}|p|^{-2}\exp(ip(x_i-x_j)),$$

in which the $p\neq 0$ condition is supposed to make up for the background that is not explicitly included in H'. It is 'physically clear' that this device works, but a rigorous proof of it is not easy.

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).

$$H' = \sum_{p} |p|^2 a_p^* a_p + \sum_{p\neq 0} L^{-3}|p|^{-2}\sum_{k,q} a_{k+p}^* a_{q-p}^* a_q a_k,$$

where the a_p operators satisfy the usual bosonic commutation relations. An important observation is that since $p\neq 0$ there are no terms with 3 or 4 $a_0^\sharp$. This is different from the situation with the usual short range potential treated in Section 2, and it means that the leading term in perturbation theory vanishes. Everything now comes from the terms with two $a_0^\sharp$.

6.1.1. *The Bogolubov approximation:* The motivation is Bose condensation: Almost all particles are in the state of momentum $p=0$ created by a_0^*. Thus:

Step 1 in the Bogolubov approximation: Keep only quartic terms with precisely two $a_0^\sharp$ (and ignore terms with one or no $a_0^\sharp$). We obtain the reduced Hamiltonian

$$\begin{aligned} H'' \;=\; & \sum_{p} |p|^2 a_p^* a_p + \sum_{p\neq 0} L^{-3}|p|^{-2}\Big[a_p^* a_0^* a_p a_0 \\ & + a_0^* a_{-p}^* a_0 a_{-p} + a_p^* a_{-p}^* a_0 a_0 + a_0^* a_0^* a_p a_{-p}\Big] \end{aligned}$$

Step 2 in the Bogolubov approximation: Replace the *operators* $a_0^\sharp$ by the number $\sqrt{N}$. We then obtain:

$$\begin{aligned} H''' = \sum_{p\neq 0} \; & |p|^2 a_p^* a_p + \rho|p|^{-2}\Big[a_p^* a_p + a_{-p}^* a_{-p} \\ & + a_p^* a_{-p}^* + a_p a_{-p}\Big] \end{aligned}$$

This is a quadratic Hamiltonian and can be diagonalized by completing the square:

$$\begin{aligned} H''' &= \sum_p A_p(a_p^* + \beta_p a_{-p})(a_p + \beta_p a_{-p}^*) \\ &\quad + A_p(a_{-p}^* + \beta_p a_p)(a_{-p} + \beta_p a_p^*) \\ &\quad - 2\sum_{p\neq 0} A_p \beta_p^2 \end{aligned}$$

The last term comes from the commutator $[a_p, a_q^*] = \delta_{pq}$.

$$\begin{aligned} A_p(1+\beta_p^2) &= \frac{1}{2}|p|^2 + \rho|p|^{-2} \\ 2A_p\beta_p &= \rho|p|^{-2} \end{aligned}$$

The ground state energy is given by the last term above.

$$e = \lim_{L\to\infty} -\frac{2}{L^3}\sum_{p\neq 0} A_p\beta_p^2 = \int A_p\beta_p^2 = C_F\rho^{5/4}.$$

In this approximation the ground state wave function ψ satisfies

$$(a_p + \beta_p a_{-p}^*)\psi = 0,$$

for all $p \neq 0$.

In the original language (in which a_0 an operator) this corresponds to a function of the form

$$\begin{aligned} \psi &= 1 + \sum_{i<j} f(x_i - x_j) \\ &\quad + c \sum_{\substack{i,j,l,k \\ \text{different}}} f(x_i - x_j) f(x_l - x_k) + \dots \end{aligned}$$

where $\hat{f}(p) = \beta_p$. In fact, $\hat{f}(p) = G(|p|^4/\rho)$, with G independent of ρ. Thus f varies on a length scale $\rho^{-1/4}$ (which is the typical inter*pair* distance).

6.1.2. *Ideas in the rigorous proof:* As in the short range case in Section 2, there is no need to prove Bose condensation globally. It is enough to do so on a short scale.

- Localize particles, by means of Neumann bracketing, in "small" boxes of size ℓ. The constant function (i.e., the 'condensate') is not affected by this localization since the constant function in a small box satisfies Neumann boundary conditions. The function f discussed above is not affected very much if $\ell \gg \rho^{-1/4}$. We choose ℓ close to $\rho^{-1/4}$.
- We control the Coulomb interaction between boxes by using an averaging method in [**24**]. The error in neglecting intercell interactions can be shown to be dominated by $N/\ell \ll N\rho^{1/4}$.
- We establish condensation on the scale ℓ by noting that the first non-zero Neumann eigenvalue is $\sim \ell^{-2}$. If N_+ is the expected number N_+ of particles not in the condensate in the "small box", their energy is bounded from below by $N_+\ell^{-2} \sim N_+\rho^{1/2}$. If this is to be consistent with the total energy $-N\rho^{1/4}$ we should expect to have $N_+ \ll N\rho^{-1/4}$, i.e., local condensation exists.
- This is established by means of a bootstrap procedure.

- Having established local condensation one starts the hard work of proving that the Bogolubov 'quadratic' approximation really gives the leading term in the energy. There is however a new difficulty that arises from the finite size of the small boxes in which we are working. Neumann, and not periodic boundary conditions must be used. Since we no longer have 'momentum conservation' in the small boxes, diagonalization of the Hamiltonian by 'completing the square' is not the simple algebraic problem it was before.
- Nevertheless, it can all be carried to a succesful conclusion

References

[1] E.H. Lieb, J. Yngvason, *Ground State Energy of the low density Bose Gas*, Phys. Rev. Lett. **80**, 2504–2507 (1998). arXiv math-ph/9712138, mp_arc 97-631

[2] E.H. Lieb, J. Yngvason, *The Ground State Energy of a Dilute Two-dimensional Bose Gas*, J. Stat. Phys. (in press) arXiv math-ph/0002014, mp_arc 00-63.

[3] E.H. Lieb, R. Seiringer, and J. Yngvason, *Bosons in a Trap: A Rigorous Derivation of the Gross-Pitaevskii Energy Functional*, Phys. Rev A **61**, 043602-1 – 043602-13 (2000)mp_arc 99-312, arXiv math-ph/9908027 (1999).

[4] E.H. Lieb, R. Seiringer and J. Yngvason, *A Rigorous Derivation of the Gross-Pitaevskii Energy Functional for a Two-dimensional Bose Gas.* arXiv cond-mat/0005026, mp_arc 00-203.

[5] E.H. Lieb, J.P. Solovej, *Ground State Energy of the One-Component Charged Bose Gas.* arXiv cond-mat/0007425, mp_arc 00-303.

[6] E.H. Lieb, J. Yngvason, *The Ground State Energy of a Dilute Bose Gas*, in *Differential Equations and Mathematical Physics, University of Alabama, Birmingham, 1999*, R. Weikard and G. Weinstein, eds., 271-282 Amer. Math. Soc./Internat. Press (2000). arXiv math-ph/9910033, mp_arc 99-401.

[7] E.H. Lieb, R. Seiringer, J. Yngvason, *The Ground State Energy and Density of Interacting Bosons in a Trap*, in *Quantum Theory and Symmetries*, Goslar, 1999, H.-D. Doebner, V.K. Dobrev, J.-D. Hennig and W. Luecke, eds., pp. 101-110, World Scientific (2000). arXiv math-ph/9911026, mp_arc 99-439.

[8] W. Ketterle, N. J. van Druten, *Evaporative Cooling of Trapped Atoms*, in B. Bederson, H. Walther, eds., Advances in Atomic, Molecular and Optical Physics, **37**, 181–236, Academic Press (1996).

[9] F. Dalfovo, S. Giorgini, L.P. Pitaevskii, and S. Stringari, *Theory of Bose-Einstein condensation in trapped gases*, Rev. Mod. Phys. **71**, 463–512 (1999).

[10] R. Seiringer, Diplom thesis, University of Vienna, (1999).

[11] N.N. Bogolubov, J. Phys. (U.S.S.R.) **11**, 23 (1947); N.N. Bogolubov and D.N. Zubarev, Sov. Phys.-JETP **1**, 83 (1955).

[12] K. Huang, C.N. Yang, Phys. Rev. **105**, 767-775 (1957); T.D. Lee, K. Huang, and C.N. Yang, Phys. Rev. **106**, 1135-1145 (1957); K.A. Brueckner, K. Sawada, Phys. Rev. **106**, 1117-1127, 1128-1135 (1957).; S.T. Beliaev, Sov. Phys.-JETP **7**, 299-307 (1958); T.T. Wu, Phys. Rev. **115**, 1390 (1959); N. Hugenholtz, D. Pines, Phys. Rev. **116**, 489 (1959); M. Girardeau, R. Arnowitt, Phys. Rev. **113**, 755 (1959); T.D. Lee, C.N. Yang, Phys. Rev. **117**, 12 (1960).

[13] E.H. Lieb, *Simplified Approach to the Ground State Energy of an Imperfect Bose Gas*, Phys. Rev. **130** (1963), 2518–2528. See also Phys. Rev. **133** (1964), A899–A906 (with A.Y. Sakakura) and Phys. Rev. **134** (1964), A312–A315 (with W. Liniger).

[14] E.H. Lieb, *The Bose fluid*, in W.E. Brittin, ed., Lecture Notes in Theoretical Physics VIIC, Univ. of Colorado Press, pp. 175–224 (1964).

[15] F.J. Dyson, *Ground-State Energy of a Hard-Sphere Gas*, Phys. Rev. **106**, 20–24 (1957).

[16] B. Baumgartner, *The Existence of Many-particle Bound States Despite a Pair Interaction with Positive Scattering Length*, J. Phys. A **30** (1997), L741–L747.

[17] E.H. Lieb, W. Liniger, *Exact Analysis of an Interacting Bose Gas. I. The General Solution and the Ground State*, Phys. Rev. **130**, 1605-1616 (1963); E.H. Lieb, *Exact Analysis of an Interacting Bose Gas. II. The Excitation Spectrum*, Phys. Rev. **130**, 1616-1624 (1963).

[18] G. Temple, *The theory of Rayleigh's Principle as Applied to Continuous Systems*, Proc. Roy. Soc. London A **119** (1928), 276–293.

[19] M. Schick, *Two-Dimensional System of Hard Core Bosons*, Phys. Rev. A **3**, 1067-1073 (1971).

[20] T. Kennedy, E.H. Lieb, S. Shastry, The XY Model has Long-Range Order for all Spins and all Dimensions Greater than One, Phys. Rev. Lett. textbf 61, 2582-2584 (1988).

[21] E.H. Lieb, H. Narnhofer, *The Thermodynamic Limit for Jellium*, J. Stat. Phys. **12**, 291-310 (1975). Errata J. Stat. Phys. **14**, 465 (1976).

[22] L.L. Foldy, *Charged Boson Gas*, Phys. Rev. **124**, 649-651 (1961); Errata *ibid* **125**, 2208 (1962).

[23] F.J. Dyson, *Ground State Energy of a Finite System of Charged Particles*, J. Math. Phys. **8**, 1538-1545 (1967).

[24] J. Conlon, E.H. Lieb, H-T. Yau *The $N^{7/5}$ Law for Charged Bosons*, Commun. Math. Phys. **116**, 417-448 (1988).

[25] G.M. Graf, J.P. Solovej, *A correlation estimate with applications to quantum systems with Coulomb interactions*, Rev. Math. Phys., 6 (No. 5a, Special Issue) 977-997 (1994). mp_arc 93-60.

Departments of Mathematics and Physics, Princeton University, Princeton, New Jersey 08544-0708

E-mail address: lieb@princeton.edu