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# The Quantum-Mechanical Many-Body Problem: The Bose Gas

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**Summary.** Now that the low temperature properties of quantum-mechanical many-body systems (bosons) at low density,  $\rho$ , can be examined experimentally it is appropriate to revisit some of the formulas deduced by many authors 4–5 decades ago, and to explore new regimes not treated before. 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 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, several 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 and su-

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perfluidity, as we have shown. On the frontier of experimental developments is the possibility that a dilute gas in an elongated trap will behave like a one-dimensional system; we have proved this mathematically. 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; using this we can also prove the  $N^{7/5}$  formula for the ground state energy of the two-component charged Bose gas proposed by Dyson in 1967. 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 "Perspectives in Analysis" at the KTH, Stockholm, June 23, 2003, one of us (E.H.L.) contributed a talk with the title above. This talk covered material by all the authors listed above. This contribution is a much expanded version of the talk and of [47]. It is based on, but supersedes, the article [52].<sup>1</sup>

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<sup>1</sup> Note added in proof: A more extensive version of these notes, together with developments obtained after submission of the manuscript, recently appeared in the book: E.H. Lieb, R. Seiringer, J.P. Solovej and J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, vol. **34**, Oberwolfach Seminars Series, Birkhäuser (2005).

## 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  $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$  is automatically symmetric in the coordinates  $\mathbf{x}_j \in \mathbb{R}^3$  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 five 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 condensation and superfluidity for dilute trapped gases.
4. One-dimensional behavior of three-dimensional gases in elongated traps.
5. Foldy's “jellium” model of charged particles in a neutralizing background and the extension to the two-component gas.

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 [62] and [63], and of topic 2 on [53] and [54]. See also [64, 55, 78, 56].

The original references for topic 3 are [51] and [57], 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 inhomogeneity of the gas in a general trap. An essential technical tool for topic 3 is a generalized Poincaré inequality, which is discussed in a separate section.

Topic 4 is a summary of the work in [58].

The discussion of topic 5 is based on [60] and [61].

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 [64]. In terms of technical complexity, however, the fifth 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 5 is the repulsive, *long-range* Coulomb potential, while in topics 1–4 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 [69]. 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 interaction 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  $\Lambda$  of side length  $L$  and interacting by a spherically symmetric pair potential  $v(|\mathbf{x}_i - \mathbf{x}_j|)$ :

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

Here  $\mathbf{x}_i \in \mathbb{R}^3$ ,  $i = 1, \dots, N$  are the positions of the particles,  $\Delta_i$  the Laplacian with respect to  $\mathbf{x}_i$ , and we have denoted  $\hbar^2/2m$  by  $\mu$  for short. (By choosing suitable units  $\mu$  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  $L^2(\Lambda^N, d\mathbf{x}_1 \cdots d\mathbf{x}_N)$  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

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

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 [53]. 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  $|\mathbf{x}| = r \rightarrow \infty$  (or for all  $r > R_0$  if  $v(r) = 0$  for  $r > R_0$ ),

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

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

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

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).**

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

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 [63].

The genesis of an understanding of  $e_0(\rho)$  was the pioneering work [7] of Bogolubov, and in the 50's and early 60's several derivations of (2.8) were presented [36], [44], even including higher order terms:

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

These early developments are reviewed in [45]. 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 [17]:

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

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  $\ell_c$  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  $\ell_c$ . We then have the relation (since  $\rho a^3$  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  $\rho$  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.,  $\ell_c$  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 *is 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 [3].) 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  $\psi_0$  the zero energy scattering solution, partial integration, using (2.3) and (2.4), gives, for  $R \geq R_0$ ,

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

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  $\psi_0(|\mathbf{x}| = R) = (1 - a/R)$ . 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  $E_0(N, L) \approx N(N-1)/(2L^3) \int v(|\mathbf{x}|) d\mathbf{x}$ . In particular it is *independent of  $\mu$* , i.e. of Planck’s constant and mass. Since, however,  $\int v(|\mathbf{x}|) d\mathbf{x}$  is the first Born approximation to  $8\pi\mu a$  (note that  $a$  depends on  $\mu$ !), 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 [7] presupposes the existence of Bose–Einstein condensation. Nevertheless, it is correct (for the energy) for the one-dimensional delta-function Bose gas [48], despite the fact that there is (presumably) no condensation in that case [72]. 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 2.1 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 [17].

## 2.1 Upper Bound

The following generalization of Dyson's upper bound holds [53], [77]:

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

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

*Thus in the thermodynamic limit (and for all boundary conditions)*

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

*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

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

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

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = F_1(\mathbf{x}_1)F_2(\mathbf{x}_1, \mathbf{x}_2) \cdots F_N(\mathbf{x}_1, \dots, \mathbf{x}_N). \quad (2.17)$$

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

$$F_i(\mathbf{x}_1, \dots, \mathbf{x}_i) = f(t_i), \quad t_i = \min(|\mathbf{x}_i - \mathbf{x}_j|, j = 1, \dots, i-1), \quad (2.18)$$

with a function  $f$  satisfying

$$0 \leq f \leq 1, \quad f' \geq 0. \quad (2.19)$$

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  $\prod_{i < j} f(|\mathbf{x}_i - \mathbf{x}_j|)$ , which might appear more natural in view of the heuristic remarks after (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 [17], but making use of (2.13). For details we refer to [53] and [77]. □

### 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’  $\ell_c$ , 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  $Y \rightarrow 0$ .

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 [77].

As mentioned at the beginning of this section after (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*

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

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,  $N > (\text{const.})Y^{-1/17}$ .) 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  $\psi$*

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

*Proof.* Actually, (2.23) holds with  $\mu|\nabla\psi(\mathbf{x})|^2$  replaced by the (smaller) radial kinetic energy,  $\mu|\partial\psi(\mathbf{x})/\partial r|^2$ , 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  $\psi(\mathbf{x}) = u(r)/r$  with  $u(0) = 0$ . We consider first the special case 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

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

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 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,

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

$$\geq \mu a |R - a|^2 / R^2 .$$

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  $\delta$ -functions,  $U(r) = \int R^{-2} \delta(r - R) U(R) R^2 dR$ , and  $\int U(R) R^2 dR \leq 1$  by assumption.  $\square$

By dividing  $\Lambda$  for given points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  into Voronoi cells  $\mathcal{B}_i$  that contain all points closer to  $\mathbf{x}_i$  than to  $\mathbf{x}_j$  with  $j \neq i$  (these cells are star shaped w.r.t.  $\mathbf{x}_i$ , indeed convex), the following corollary of Lemma 2.5 can be derived in the same way as the corresponding Eq. (28) in [17].

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

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

with  $W$  the multiplication operator

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

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

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

(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  $\mathbf{x}_j$  with  $j \leq i - 1$ .)

Dyson considers in [17] 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

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

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

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

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

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

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  $|\mathbf{x}_i - \mathbf{x}_j|$  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  $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1 - \varepsilon)H_N \geq \varepsilon T_N + (1 - \varepsilon)H_N \quad (2.34)$$

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

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

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

The ground state of  $H_0$  in a box of side length  $L$  is  $\Psi_0(\mathbf{x}_1, \dots, \mathbf{x}_N) \equiv L^{-3N/2}$  and we denote expectation values in this state by  $\langle \cdot \rangle_0$ . A computation, cf. Eq. (21) in [62] (see also (3.15)–(3.20)), gives

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

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  $\Lambda$ , 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  $L \rightarrow \infty$ ,  $N \rightarrow \infty$  with  $\rho = N/L^3$  fixed, and subsequently take  $R \rightarrow 0$ , 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  $\varepsilon$ ,  $R$  and  $L$ .

We now recall *Temple's inequality* [83] 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

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

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 Schwarz inequality. A glance at the form of the error term reveals, however, that it is *not* possible here to take the thermodynamic limit  $L \rightarrow \infty$  with  $\rho$  fixed: We have  $E_1^{(0)} = \varepsilon\pi^2\mu/L^2$  (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 loses its validity if  $L$  is large enough.

As a way out of this dilemma we divide the big box  $\Lambda$  into cubic *cells* of side length  $\ell$  that is kept *fixed* as  $L \rightarrow \infty$ . The number of cells,  $L^3/\ell^3$ , on the other hand, increases with  $L$ . The  $N$  particles are distributed among these cells, and we use (2.40), with  $L$  replaced by  $\ell$ ,  $N$  by the particle number,  $n$ , in a cell and  $\rho$  by  $n/\ell^3$ , 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

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

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

$$\sum_{n \geq 0} c_n = 1, \quad \sum_{n \geq 0} c_n n = \rho\ell^3. \quad (2.43)$$

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

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

i.e., replacement of  $L$  in (2.39) by  $\ell$ , which is independent of  $L$ . The blow up of  $\mathcal{E}$  for  $L \rightarrow \infty$  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

$$E_0(n + n', \ell) \geq E_0(n, \ell) + E_0(n', \ell) \quad (2.45)$$

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  $n \geq p$

$$E_0(n, \ell) \geq [n/p] E_0(p, \ell) \geq \frac{n}{2p} E_0(p, \ell) \quad (2.46)$$

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  $\ell$ ,  $N$  by  $n$  and  $\rho$  by  $n/\ell^3$  in (2.39) we have for fixed  $R$  and  $\varepsilon$

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

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

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

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

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

subject to the constraints (2.43). Putting

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

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

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

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

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

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

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

The estimate (2.47) with this  $K$  is valid as long as the denominator in the last factor in (2.53) is  $\geq 0$ , 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

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

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 forgotten. We now make the ansatz

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

with exponents  $\alpha$ ,  $\beta$  and  $\gamma$  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  $\varepsilon \rightarrow 0$  for  $Y \rightarrow 0$ .
- $3\beta - 1 > 0$  in order that  $Y^{-1}(a/\ell)^3 \rightarrow 0$  for  $Y \rightarrow 0$ .
- $1 - 3\beta + \gamma > 0$  in order that  $Y(\ell/a)^3(R^3 - R_0^3)/\ell^3 \rightarrow 0$  for  $Y \rightarrow 0$ .
- $1 - \alpha - 2\beta - \gamma > 0$  to control the last factor in (2.54).

Taking

$$\alpha = 1/17, \quad \beta = 6/17, \quad \gamma = 3/17 \quad (2.57)$$

all these conditions are satisfied, and

$$\alpha = 3\beta - 1 = 1 - 3\beta + \gamma = 1 - \alpha - 2\beta - \gamma = 1/17. \quad (2.58)$$

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 [77]. 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 [63] and Appendix B in [53] for details. We remark that a slower decrease of the potential than  $1/r^3$  implies infinite scattering length.  $\square$

The exponents (2.57) mean in particular that

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

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  $\gg e_0(\rho)$  in Temple's inequality. It is also clear that this choice of  $\ell$  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 [75] for a gas of hard discs. He found



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

This was accomplished by an infinite summation of ‘perturbation series’ diagrams. Subsequently, a corrected modification of [75] was given in [32]. Positive temperature extensions were given in [73] and in [22]. 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 [44]. Ovchinnikov [68] derived (3.1) by using, basically, the method in [44]. 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 [63].

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  $\rho$ , 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  $8\pi\mu L^{-2} [\ln(L^2/a^2)]^{-1}$ . (This is seen in an analogous way as (2.13). The three-dimensional boundary condition  $\psi_0(|\mathbf{x}| = R) = 1 - a/R$  is replaced by  $\psi_0(|\mathbf{x}| = R) = \ln(R/a)$  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  $4\pi\mu\rho [\ln(L^2/a^2)]^{-1}$ . In other words,  $L$ , which tends to  $\infty$  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.

Equation (3.1) was proved in [63] 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  $O(|\ln(\rho a^2)|^{-1})$  while the lower bound will have remainder  $O(|\ln(\rho a^2)|^{-1/5})$ . It is claimed in [32] that the relative error for a hard core gas is negative and  $O(\ln|\ln(\rho a^2)||\ln(\rho a^2)|^{-1})$ , 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

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

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

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

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*

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

*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  $\psi$  in the Sobolev space  $H^1(\mathcal{B})$ ,*

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

*Proof.* In polar coordinates,  $r, \theta$ , 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  $f(r)$ ,

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

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

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

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

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  $\mathcal{D}_R = \{\mathbf{x} \in \mathbb{R}^2 : 0 \leq |\mathbf{x}| \leq R\}$ . (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

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

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  $R(\theta)$ .  $\square$

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  $0 < \varepsilon < 1$*

$$H_N \geq \varepsilon T_N + (1 - \varepsilon)\mu W \quad (3.9)$$

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

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

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

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

with  $\nu(R)$  chosen so that

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

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

$$\begin{aligned} \nu(R) &= \int_{R_0}^R \ln(r/a) r dr \\ &= \frac{1}{4} \left\{ R^2 (\ln(R^2/a^2) - 1) - R_0^2 (\ln(R_0^2/a^2) - 1) \right\} . \end{aligned} \quad (3.13)$$

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

As in Sect. 2.2 we shall need estimates on the expectation value,  $\langle W_R \rangle_0$ , of  $W_R$  in the ground state of  $\varepsilon T_N$  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

$$A(R) = \pi(R^2 - R_0^2). \quad (3.14)$$

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  $\ell$  are obtained by the same geometric reasoning as lead to (2.36), cf. [62]:

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

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

with

$$Q = A(R)/\ell^2 \quad (3.17)$$

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

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

As in [62] we estimate  $[1 - (1 - Q)^{(n-1)}]$  by

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

This gives

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

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

From Temple's inequality [83] we obtain like in (2.38) the estimate

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

where

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

is the energy of the lowest excited state of  $\varepsilon T_n$ . This estimate is valid for  $E_1^{(0)}/\mu > \langle W_R \rangle_0$ , i.e., it is important that  $\ell$  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

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

Note that  $Q$  depends on  $\ell$  and  $R$ , and  $K$  depends on  $\ell$ ,  $R$  and  $\varepsilon$  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  $\ell$ :

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

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

Let us now look at the conditions on the parameters  $\varepsilon$ ,  $R$  and  $\ell$  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

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

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

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

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*

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

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

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

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

where  $e_0(\rho) = \lim_{N \rightarrow \infty} E_0(N, \rho^{-1/2} N^{1/2})/N$ . 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 Generalized Poincaré Inequalities

This section contains some lemmas that are of independent mathematical interest, but whose significance for the physics of the Bose gas may not be obvious at this point. They will, however, turn out to be important tools for the discussion of Bose–Einstein condensation (BEC) and superfluidity in the next section.

The classic Poincaré inequality [49] bounds the  $L^q$ -norm of a function,  $f$ , orthogonal to a given function  $g$  in a domain  $\mathcal{K}$ , in terms of some  $L^p$ -norm of its gradient in  $\mathcal{K}$ . For the proof of BEC we shall need a generalization of this inequality where the estimate is in terms of the gradient of  $f$  on a subset  $\Omega \subset \mathcal{K}$  and a remainder that tends to zero with the volume of the complement  $\Omega^c = \mathcal{K} \setminus \Omega$ . For superfluidity it will be necessary to generalize this further by adding a vector potential to the gradient. This is the most complex of the lemmas because the other two can be derived directly from the classical Poincaré inequality using Hölder’s inequality. The first lemma is the simplest variant and it is sufficient for the discussion of BEC in the case of a homogeneous gas. In this case the function  $g$  can be taken to be the constant function. The same holds for the second lemma, which will be used for the discussion of superfluidity in a homogeneous gas with periodic

boundary conditions, but the modification of the gradient requires a more elaborate proof. The last lemma, that will be used for the discussion of BEC in the inhomogeneous case, is again a simple consequence of the classic Poincaré and Hölder inequalities. For a more comprehensive discussion of generalized Poincaré inequalities with further generalizations we refer to [59].

**Lemma 4.1 (Generalized Poincaré inequality: Homogeneous case).** *Let  $\mathcal{K} \subset \mathbb{R}^3$  be a cube of side length  $L$ , and define the average of a function  $f \in L^1(\mathcal{K})$  by*

$$\langle f \rangle_{\mathcal{K}} = \frac{1}{L^3} \int_{\mathcal{K}} f(\mathbf{x}) \, d\mathbf{x} . \tag{4.1}$$

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

$$\int_{\mathcal{K}} |f(\mathbf{x}) - \langle f \rangle_{\mathcal{K}}|^2 d\mathbf{x} \leq C \left( L^2 \int_{\Omega} |\nabla f(\mathbf{x})|^2 d\mathbf{x} + |\Omega^c|^{2/3} \int_{\mathcal{K}} |\nabla f(\mathbf{x})|^2 d\mathbf{x} \right) \tag{4.2}$$

*holds. Here  $\Omega^c = \mathcal{K} \setminus \Omega$ , 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  $\mathcal{K}$  (see [49], Thm. 8.12), we infer that there exists a  $C > 0$  such that

$$\begin{aligned} \|f - \langle f \rangle_{\mathcal{K}}\|_{L^2(\mathcal{K})}^2 &\leq \frac{1}{2} C \|\nabla f\|_{L^{6/5}(\mathcal{K})}^2 \\ &\leq C \left( \|\nabla f\|_{L^{6/5}(\Omega)}^2 + \|\nabla f\|_{L^{6/5}(\Omega^c)}^2 \right) . \end{aligned} \tag{4.3}$$

Applying Hölder’s inequality

$$\|\nabla f\|_{L^{6/5}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} |\Omega|^{1/3} \tag{4.4}$$

(and the analogue with  $\Omega$  replaced by  $\Omega^c$ ), we see that (4.2) holds.  $\square$

In the next lemma  $\mathcal{K}$  is again a cube of side length  $L$ , but we now replace the gradient  $\nabla$  by

$$\nabla_{\varphi} := \nabla + i(0, 0, \varphi/L) , \tag{4.5}$$

where  $\varphi$  is a real parameter, and require periodic boundary conditions on  $\mathcal{K}$ .

**Lemma 4.2 (Generalized Poincaré inequality with a vector potential).** *For any  $|\varphi| < \pi$  there are constants  $c > 0$  and  $C < \infty$  such that for all subsets  $\Omega \subset \mathcal{K}$  and all functions  $f \in H^1(\mathcal{K})$  with periodic boundary conditions on  $\mathcal{K}$  the following estimate holds:*

$$\begin{aligned} \|\nabla_{\varphi} f\|_{L^2(\Omega)}^2 &\geq \frac{\varphi^2}{L^2} \|f\|_{L^2(\mathcal{K})}^2 + \frac{c}{L^2} \|f - \langle f \rangle_{\mathcal{K}}\|_{L^2(\mathcal{K})}^2 \\ &\quad - C \left( \|\nabla_{\varphi} f\|_{L^2(\mathcal{K})}^2 + \frac{1}{L^2} \|f\|_{L^2(\mathcal{K})}^2 \right) \left( \frac{|\Omega|^c}{L^3} \right)^{1/2} . \end{aligned} \tag{4.6}$$

*Here  $|\Omega^c|$  is the volume of  $\Omega^c = \mathcal{K} \setminus \Omega$ , the complement of  $\Omega$  in  $\mathcal{K}$ .*

*Proof.* We shall derive (4.6) from a special form of this inequality that holds for all functions that are orthogonal to the constant function. Namely, for any positive  $\alpha < 2/3$  and some constants  $c > 0$  and  $\tilde{C} < \infty$  (depending only on  $\alpha$  and  $|\varphi| < \pi$ ) we claim that

$$\|\nabla_\varphi h\|_{L^2(\Omega)}^2 \geq \frac{\varphi^2 + c}{L^2} \|h\|_{L^2(\mathcal{K})}^2 - \tilde{C} \left( \frac{|\Omega^c|}{L^3} \right)^\alpha \|\nabla_\varphi h\|_{L^2(\mathcal{K})}^2, \quad (4.7)$$

provided  $\langle 1, h \rangle_{\mathcal{K}} = 0$ . (Remark: Equation (4.7) holds also for  $\alpha = 2/3$ , but the proof is slightly more complicated in that case. See [59].) If (4.7) is known the derivation of (4.6) is easy: For any  $f$ , the function  $h = f - L^{-3} \langle 1, f \rangle_{\mathcal{K}}$  is orthogonal to 1. Moreover,

$$\begin{aligned} \|\nabla_\varphi h\|_{L^2(\Omega)}^2 &= \|\nabla_\varphi h\|_{L^2(\mathcal{K})}^2 - \|\nabla_\varphi h\|_{L^2(\Omega^c)}^2 \\ &= \|\nabla_\varphi f\|_{L^2(\Omega)}^2 - \frac{\varphi^2}{L^2} |\langle L^{-3/2}, f \rangle_{\mathcal{K}}|^2 \left( 1 + \frac{|\Omega^c|}{L^3} \right) \\ &\quad + 2 \frac{\varphi}{L} \operatorname{Re} \langle L^{-3/2}, f \rangle_{\mathcal{K}} \langle \nabla_\varphi f, L^{-3/2} \rangle_{\Omega^c} \\ &\leq \|\nabla_\varphi f\|_{L^2(\Omega)}^2 - \frac{\varphi^2}{L^2} |\langle L^{-3/2}, f \rangle_{\mathcal{K}}|^2 \\ &\quad + \frac{|\varphi|}{L} \left( L \|\nabla_\varphi f\|_{L^2(\mathcal{K})}^2 + \frac{1}{L} \|f\|_{L^2(\mathcal{K})}^2 \right) \left( \frac{|\Omega^c|}{L^3} \right)^{1/2} \end{aligned} \quad (4.8)$$

and

$$\begin{aligned} \frac{\varphi^2 + c}{L^2} \|h\|_{L^2(\mathcal{K})}^2 &= \frac{\varphi^2}{L^2} \left( \|f\|_{L^2(\mathcal{K})}^2 - |\langle L^{-3/2}, f \rangle_{\mathcal{K}}|^2 \right) \\ &\quad + \frac{c}{L^2} \|f - L^{-3} \langle 1, f \rangle_{\mathcal{K}}\|_{L^2(\mathcal{K})}^2. \end{aligned} \quad (4.9)$$

Setting  $\alpha = \frac{1}{2}$ , using  $\|\nabla_\varphi h\|_{L^2(\mathcal{K})} \leq \|\nabla_\varphi f\|_{L^2(\mathcal{K})}$  in the last term in (4.7) and combining (4.7), (4.8) and (4.9) gives (4.6) with  $C = |\varphi| + \tilde{C}$ .

We now turn to the proof of (4.7). For simplicity we set  $L = 1$ . The general case follows by scaling. Assume that (4.7) is false. Then there exist sequences of constants  $C_n \rightarrow \infty$ , functions  $h_n$  with  $\|h_n\|_{L^2(\mathcal{K})} = 1$  and  $\langle 1, h_n \rangle_{\mathcal{K}} = 0$ , and domains  $\Omega_n \subset \mathcal{K}$  such that

$$\lim_{n \rightarrow \infty} \left\{ \|\nabla_\varphi h_n\|_{L^2(\Omega_n)}^2 + C_n |\Omega_n^c|^\alpha \|\nabla_\varphi h_n\|_{L^2(\mathcal{K})}^2 \right\} \leq \varphi^2. \quad (4.10)$$

We shall show that this leads to a contradiction.

Since the sequence  $h_n$  is bounded in  $L^2(\mathcal{K})$  it has a subsequence, denoted again by  $h_n$ , that converges weakly to some  $h \in L^2(\mathcal{K})$  (i.e.,  $\langle g, h_n \rangle_{\mathcal{K}} \rightarrow \langle g, h \rangle_{\mathcal{K}}$  for all  $g \in L^2(\mathcal{K})$ ). Moreover, by Hölder's inequality the  $L^p(\Omega_n^c)$  norm  $\|\nabla_\varphi h_n\|_{L^p(\Omega_n^c)} = \left( \int_{\Omega_n^c} |\nabla_\varphi h(\mathbf{x})|^p d\mathbf{x} \right)^{1/p}$  is bounded by  $|\Omega_n^c|^{\alpha/2} \|\nabla_\varphi h_n\|_{L^2(\mathcal{K})}$  for  $p = 2/(\alpha + 1)$ . From (4.10) we conclude that  $\|\nabla_\varphi h_n\|_{L^p(\Omega_n^c)}$  is bounded and also that  $\|\nabla_\varphi h_n\|_{L^p(\Omega_n)} \leq \|\nabla_\varphi h_n\|_{L^2(\Omega_n)}$  is bounded. Altogether,  $\nabla_\varphi h_n$



is bounded in  $L^p(\mathcal{K})$ , and by passing to a further subsequence if necessary, we can therefore assume that  $\nabla_\varphi h_n$  converges weakly in  $L^p(\mathcal{K})$ . The same applies to  $\nabla h_n$ . Since  $p = 2/(\alpha + 1)$  with  $\alpha < 2/3$  the hypotheses of the Rellich–Kondrashov Theorem [49, Thm. 8.9] are fulfilled and consequently  $h_n$  converges *strongly* in  $L^2(\mathcal{K})$  to  $h$  (i.e.,  $\|h - h_n\|_{L^2(\mathcal{K})} \rightarrow 0$ ). We shall now show that

$$\liminf_{n \rightarrow \infty} \|\nabla_\varphi h_n\|_{L^2(\Omega_n)}^2 \geq \|\nabla_\varphi h\|_{L^2(\mathcal{K})}^2. \tag{4.11}$$

This will complete the proof because the  $h_n$  are normalized and orthogonal to 1 and the same holds for  $h$  by strong convergence. Hence the right side of (4.11) is necessarily  $> \varphi^2$ , since for  $|\varphi| < \pi$  the lowest eigenvalue of  $-\nabla_\varphi^2$ , with constant eigenfunction, is non-degenerate. This contradicts (4.10).

Equation (4.11) is essentially a consequence of the weak lower semicontinuity of the  $L^2$  norm, but the dependence on  $\Omega_n$  leads to a slight complication. First, (4.10) and  $C_n \rightarrow \infty$  clearly imply that  $|\Omega_n^c| \rightarrow 0$ , because  $\|\nabla_\varphi h_n\|_{L^2(\mathcal{K})}^2 > \varphi^2$ . By choosing a subsequence we may assume that  $\sum_n |\Omega_n^c| < \infty$ . For some fixed  $N$  let  $\tilde{\Omega}_N = \mathcal{K} \setminus \cup_{n \geq N} \Omega_n^c$ . Then  $\tilde{\Omega}_N \subset \Omega_n$  for  $n \geq N$ . Since  $\|\nabla_\varphi h_n\|_{L^2(\Omega_n)}$  is bounded,  $\nabla_\varphi h_n$  is also bounded in  $L^2(\tilde{\Omega}_N)$  and a subsequence of it converges weakly in  $L^2(\tilde{\Omega}_N)$  to  $\nabla_\varphi h$ . Hence

$$\liminf_{n \rightarrow \infty} \|\nabla_\varphi h_n\|_{L^2(\Omega_n)}^2 \geq \liminf_{n \rightarrow \infty} \|\nabla_\varphi h_n\|_{L^2(\tilde{\Omega}_N)}^2 \geq \|\nabla_\varphi h\|_{L^2(\tilde{\Omega}_N)}^2. \tag{4.12}$$

Since  $\tilde{\Omega}_N \subset \tilde{\Omega}_{N+1}$  and  $\cup_N \tilde{\Omega}_N = \mathcal{K}$  (up to a set of measure zero), we can now let  $N \rightarrow \infty$  on the right side of (4.12). By monotone convergence this converges to  $\|\nabla_\varphi h\|_{L^2(\mathcal{K})}^2$ . This proves (4.11) which, as remarked above, contradicts (4.10).  $\square$

The last lemma is a simple generalization of Lemma 4.1 with  $\mathcal{K} \subset \mathbb{R}^m$  a bounded and connected set that is sufficiently nice so that the Poincaré–Sobolev inequality (see [49, Thm. 8.12]) holds on  $\mathcal{K}$ . In particular, this is the case if  $\mathcal{K}$  satisfies the cone property [49] (e.g. if  $\mathcal{K}$  is a rectangular box or a cube). Moreover, the constant function on  $\mathcal{K}$  is here replaced by a more general bounded function.

**Lemma 4.3 (Generalized Poincaré inequality: Inhomog. case).** *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  $\int_{\mathcal{K}} f h \, dx = 0$ , the inequality*

$$\int_{\mathcal{K}} |f(\mathbf{x})|^2 \, dx \leq C \left( \int_{\Omega} |\nabla f(\mathbf{x})|^2 \, dx + \left( \frac{|\Omega^c|}{|\mathcal{K}|} \right)^{2/d} \int_{\mathcal{K}} |\nabla f(\mathbf{x})|^2 \, dx \right) \tag{4.13}$$

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 [49, Thm. 8.12]),

$$\begin{aligned} \|f\|_{L^2(\mathcal{K})}^2 &\leq \tilde{C} \|\nabla f\|_{L^{2d/(d+2)}(\mathcal{K})}^2 \\ &\leq 2\tilde{C} \left( \|\nabla f\|_{L^{2d/(d+2)}(\Omega)}^2 + \|\nabla f\|_{L^{2d/(d+2)}(\Omega^c)}^2 \right), \end{aligned} \quad (4.14)$$

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

$$\|\nabla f\|_{L^{2d/(d+2)}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} |\Omega|^{1/d} \quad (4.15)$$

(and the analogue with  $\Omega$  replaced by  $\Omega^c$ ), we see that (4.6) holds with  $C = 2|\mathcal{K}|^{2/d}\tilde{C}$ .  $\square$

## 5 Bose–Einstein Condensation and Superfluidity for Homogeneous Gases

### 5.1 Bose–Einstein Condensation

Bose–Einstein condensation (BEC) is the phenomenon of a macroscopic occupation of a single one-particle quantum state, discovered by Einstein for thermal equilibrium states of an ideal Bose gas at sufficiently low temperatures [20]. We are here concerned with interacting Bose gases, where the question of the existence of BEC is highly nontrivial even for the ground state. Due to the interaction the many body ground state is not a product of one-particle states but the concept of a macroscopic occupation of a single state acquires a precise meaning through the *one-particle density* matrix. Given the normalized ground state wave function this is the operator on  $L^2(\mathbb{R}^d)$  ( $d = 2$  or  $3$ ) given by the kernel

$$\gamma(\mathbf{x}, \mathbf{x}') = N \int \Psi_0(\mathbf{x}, \mathbf{X}) \Psi_0(\mathbf{x}', \mathbf{X}) d\mathbf{X}, \quad (5.1)$$

where we introduced the short hand notation

$$\mathbf{X} = (\mathbf{x}_2, \dots, \mathbf{x}_N) \quad \text{and} \quad d\mathbf{X} = \prod_{j=2}^N d\mathbf{x}_j. \quad (5.2)$$

Then  $\int \gamma(\mathbf{x}, \mathbf{x}) d\mathbf{x} = \text{Tr}[\gamma] = N$ . BEC in the ground state means, by definition, that this operator has an eigenvalue of order  $N$  in the thermodynamic limit. Since  $\gamma$  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

$$\frac{1}{L^d} \int \int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = O(N) \quad (5.3)$$

as  $N \rightarrow \infty, L \rightarrow \infty$  with  $N/L^d$  fixed; more precisely (5.3) requires that there is a  $c > 0$  such that the left side is  $> cN$  for all large  $N$ . This is also referred to as *off-diagonal long range order*. Unfortunately, this is something that is frequently invoked but has so far never been 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 [38] and [19].

The problem remains open after more than 75 years since the first investigations on the Bose gas [9, 20]. Our construction in Sect. 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  $\text{volume}^{1/3}$ . The same remark applies to the 2D case of Sect. 3, where BEC is proved over a length scale  $\rho^{-1/10}|\ln(\rho a^2)|^{1/10}$ .

In a certain limit, however, one can prove (5.3), as has been shown in [51]. 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  $1/N$ , i.e., the parameter  $Na/L$  is kept fixed. Changing  $a$  with  $N$  can be done by scaling, i.e., we write

$$v(|\mathbf{x}|) = \frac{1}{a^2}v_1(|\mathbf{x}|/a) \tag{5.4}$$

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  $N^{-2/3}$  since  $L = (N/\rho)^{1/3} \sim N^{1/3}$  for  $\rho$  fixed), 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.

We shall refer to this as the *Gross–Pitaevskii (GP) limit* since  $Na/L$  will turn out to be the natural interaction parameter for inhomogeneous Bose gases confined in traps, that are described by the Gross–Pitaevskii equation discussed in Sects. 6 and 7. Its significance for a homogeneous gas can also be seen by noting that  $Na/L$  is the ratio of  $\rho a$  to  $1/L^2$ , i.e., in the GP limit the interaction energy per particle is of the same order of magnitude as the energy gap in the box, so that the interaction is still clearly visible, even though  $a \rightarrow 0$ . Note that  $\rho a^3 \sim N^{-2}$  in the GP limit, so letting  $N \rightarrow \infty$  with  $\rho$  fixed and  $Na/L$  fixed can be regarded as a *simultaneous thermodynamic and low density limit*. For simplicity, we shall here treat only the 3D case.

**Theorem 5.1 (BEC in a dilute limit).** *Assume that, as  $N \rightarrow \infty, \rho = N/L^3$  and  $g = Na/L$  stay fixed, and impose either periodic or Neumann boundary conditions for  $H$ . Then*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \frac{1}{L^3} \int \int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = 1. \tag{5.5}$$

The reason we do not deal with Dirichlet boundary conditions at this point should be clear from the discussion preceding the theorem: There would be an additional contribution  $\sim 1/L^2$  to the energy, i.e. of the same order as

the interaction energy, and the system would not be homogeneous any more. Dirichlet boundary conditions can, however, be treated with the methods of Sect. 7.

By scaling, the limit in Theorem 5.1 is equivalent to considering a Bose gas in a *fixed box* of side length  $L = 1$ , and keeping  $Na$  fixed as  $N \rightarrow \infty$ , i.e.,  $a \sim 1/N$ . The ground state energy of the system is then, asymptotically,  $N \times 4\pi Na$ , and Theorem 5.1 implies that the one-particle reduced density matrix  $\gamma$  of the ground state converges, after division by  $N$ , to the projection onto the constant function. An analogous result holds true for inhomogeneous systems as will be discussed in Sect. 7.

The proof of Theorem 5.1 has two main ingredients. One is *localization of the energy* that is stated as Lemma 5.2 below. This lemma is a refinement of the energy estimates of Sect. 2.2 and says essentially that the kinetic energy of the ground state is concentrated in a subset of configuration space where at least one pair of particles is close together and whose volume tends to zero as  $a \rightarrow 0$ . The other is the generalized Poincaré inequality, Lemma 4.1 from which one deduces that the one particle density matrix is approximately constant if the kinetic energy is localized in a small set.

The localization lemma will be proved in a slightly more general version that is necessary for Theorem 5.1, namely with the gradient  $\nabla$  replaced by  $\nabla_\varphi = \nabla + i(0, 0, \varphi/L)$ , cf. (4.5). We denote by  $H'_N$  the corresponding many-body Hamiltonian (2.1) with  $\nabla_\varphi$  in place of  $\nabla$ . This generalization will be used in the subsequent discussion of superfluidity, but a reader who wishes to focus on Theorem 5.1 only can simply ignore the  $\varphi$  and the reference to the diamagnetic inequality in the proof. We denote the gradient with respect to  $\mathbf{x}_1$  by  $\nabla_1$ , and the corresponding modified operator by  $\nabla_{1,\varphi}$ .

**Lemma 5.2 (Localization of energy).** *Let  $\mathcal{K}$  be a box of side length  $L$ . For all symmetric, normalized wave functions  $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$  with periodic boundary conditions on  $\mathcal{K}$ , and for  $N \geq Y^{-1/17}$ ,*

$$\begin{aligned} \frac{1}{N} \langle \Psi, H'_N \Psi \rangle &\geq (1 - \text{const. } Y^{1/17}) \\ &\times \left( 4\pi\mu\rho a + \mu \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\Omega_{\mathbf{X}}} d\mathbf{x}_1 |\nabla_{1,\varphi} \Psi(\mathbf{x}_1, \mathbf{X})|^2 \right), \end{aligned} \quad (5.6)$$

where  $\mathbf{X} = (\mathbf{x}_2, \dots, \mathbf{x}_N)$ ,  $d\mathbf{X} = \prod_{j=2}^N d\mathbf{x}_j$ , and

$$\Omega_{\mathbf{X}} = \left\{ \mathbf{x}_1 : \min_{j \geq 2} |\mathbf{x}_1 - \mathbf{x}_j| \geq R \right\} \quad (5.7)$$

with  $R = aY^{-5/17}$ .

*Proof.* Since  $\Psi$  is symmetric, the left side of (5.6) can be written as

$$\int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} d\mathbf{x}_1 \left[ \mu |\nabla_{1,\varphi} \Psi(\mathbf{x}_1, \mathbf{X})|^2 + \frac{1}{2} \sum_{j \geq 2} v(|\mathbf{x}_1 - \mathbf{x}_j|) |\Psi(\mathbf{x}_1, \mathbf{X})|^2 \right]. \quad (5.8)$$

For any  $\varepsilon > 0$  and  $R > 0$  this is

$$\geq \varepsilon T + (1 - \varepsilon)(T^{\text{in}} + I) + (1 - \varepsilon)T_\varphi^{\text{out}}, \quad (5.9)$$

with

$$T = \mu \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} dx_1 |\nabla_1 |\Psi(\mathbf{x}_1, \mathbf{X})||^2, \quad (5.10)$$

$$T^{\text{in}} = \mu \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\Omega_{\mathbf{X}}^c} dx_1 |\nabla_1 |\Psi(\mathbf{x}_1, \mathbf{X})||^2, \quad (5.11)$$

$$T_\varphi^{\text{out}} = \mu \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\Omega_{\mathbf{X}}} dx_1 |\nabla_{1,\varphi} \Psi(\mathbf{x}_1, \mathbf{X})|^2, \quad (5.12)$$

and

$$I = \frac{1}{2} \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} dx_1 \sum_{j \geq 2} v(|\mathbf{x}_1 - \mathbf{x}_j|) |\Psi(\mathbf{x}_1, \mathbf{X})|^2. \quad (5.13)$$

Here

$$\Omega_{\mathbf{X}}^c = \{\mathbf{x}_1 : |\mathbf{x}_1 - \mathbf{x}_j| < R \text{ for some } j \geq 2\} \quad (5.14)$$

is the complement of  $\Omega_{\mathbf{X}}$ , and the diamagnetic inequality [49]  $|\nabla_\varphi f(\mathbf{x})|^2 \geq |\nabla |f(\mathbf{x})||^2$  has been used. The proof is completed by using the estimates used for the proof of Theorem 2.4 in particular (2.52) and (2.54)–(2.57), which tell us that for  $\varepsilon = Y^{1/17}$  and  $R = aY^{-5/17}$

$$\varepsilon T + (1 - \varepsilon)(T^{\text{in}} + I) \geq (1 - \text{const. } Y^{1/17}) 4\pi\mu\rho a \quad (5.15)$$

as long as  $N \geq Y^{-1/17}$ .  $\square$

*Proof (Theorem 5.1).* We combine Lemma 5.2 (with  $\varphi = 0$  and hence  $H'_N = H_N$ ) with Lemma 4.1 that gives a lower bound to the second term on the right side of (5.6). We thus infer that, for any symmetric  $\Psi$  with  $\langle \Psi, \Psi \rangle = 1$  and for  $N$  large enough,

$$\begin{aligned} & \frac{1}{N} \langle \Psi, H_N \Psi \rangle (1 - \text{const. } Y^{1/17})^{-1} \\ & \geq 4\pi\mu\rho a - CY^{1/17} \left( \frac{1}{L^2} - \frac{1}{N} \langle \Psi, \sum_j \nabla_j^2 \Psi \rangle \right) \\ & \quad + \frac{c}{L^2} \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} dx_1 \left| \Psi(\mathbf{x}_1, \mathbf{X}) - L^{-3} [\int_{\mathcal{K}} dx \Psi(\mathbf{x}, \mathbf{X})] \right|^2, \end{aligned} \quad (5.16)$$

where we used that  $|\Omega^c| \leq \frac{4\pi}{3} NR^3 = \text{const. } L^3 Y^{2/17}$ . Since the kinetic energy, divided by  $N$ , is certainly bounded independent of  $N$ , as the upper bound (2.14) shows, and since the upper and the lower bound to  $E_0$  agree in the limit considered, the positive last term in (5.16) has to vanish in the limit. I.e., we get that for the ground state wave function  $\Psi_0$  of  $H_N$

$$\lim_{N \rightarrow \infty} \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} dx_1 \left| \Psi_0(\mathbf{x}_1, \mathbf{X}) - L^{-3} [\int_{\mathcal{K}} dx \Psi_0(\mathbf{x}, \mathbf{X})] \right|^2 = 0. \quad (5.17)$$

This proves (5.5), since

$$\begin{aligned} \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} dx_1 \left| \Psi_0(\mathbf{x}_1, \mathbf{X}) - L^{-3} \left[ \int_{\mathcal{K}} dx \Psi_0(\mathbf{x}, \mathbf{X}) \right] \right|^2 \\ = 1 - \frac{1}{NL^3} \int_{\mathcal{K} \times \mathcal{K}} \gamma(\mathbf{x}, \mathbf{x}') dx dx'. \end{aligned} \quad (5.18)$$

□

## 5.2 Superfluidity

The phenomenological two-fluid model of superfluidity (see, e.g., [84]) is based on the idea that the particle density  $\rho$  is composed of two parts, the density  $\rho_s$  of the inviscid superfluid and the normal fluid density  $\rho_n$ . If an external velocity field is imposed on the fluid (for instance by moving the walls of the container) only the viscous normal component responds to the velocity field, while the superfluid component stays at rest. In accord with these ideas the superfluid density in the ground state is often defined as follows [34]: Let  $E_0$  denote the ground state energy of the system in the rest frame and  $E'_0$  the ground state energy, measured in the moving frame, when a velocity field  $\mathbf{v}$  is imposed. Then for small  $\mathbf{v}$

$$\frac{E'_0}{N} = \frac{E_0}{N} + (\rho_s/\rho) \frac{1}{2} m \mathbf{v}^2 + O(|\mathbf{v}|^4) \quad (5.19)$$

where  $N$  is the particle number and  $m$  the particle mass. At positive temperatures the ground state energy should be replaced by the free energy. (Remark: It is important here that (5.19) holds uniformly for all large  $N$ ; i.e., that the error term  $O(|\mathbf{v}|^4)$  can be bounded independently of  $N$ . For fixed  $N$  and a finite box, (5.19) with  $\rho_s/\rho = 1$  always holds for a Bose gas with an arbitrary interaction if  $\mathbf{v}$  is small enough, owing to the discreteness of the energy spectrum.<sup>2</sup>) There are other definitions of the superfluid density that may lead to different results [74], but this is the one we shall use here and shall not dwell on this issue since it is not clear that there is a “one-size-fits-all” definition of superfluidity. For instance, in the definition we use here the ideal Bose gas is a perfect superfluid in its ground state, whereas the definition of Landau in terms of a linear dispersion relation of elementary excitations would indicate otherwise. Our main result is that with the definition adopted here there

<sup>2</sup> The ground state with  $\mathbf{v} = 0$  remains an eigenstate of the Hamiltonian with arbitrary  $\mathbf{v}$  (but not necessarily a ground state) since its total momentum is zero. Its energy is  $\frac{1}{2} m N \mathbf{v}^2$  above the ground state energy for  $\mathbf{v} = 0$ . Since in a finite box the spectrum of the Hamiltonian for arbitrary  $\mathbf{v}$  is discrete and the energy gap above the ground state is bounded away from zero for  $\mathbf{v}$  small, the ground state for  $\mathbf{v} = 0$  is at the same time the ground state of the Hamiltonian with  $\mathbf{v}$  if  $\frac{1}{2} m N \mathbf{v}^2$  is smaller than the gap.

is 100% superfluidity in the ground state of a 3D Bose gas in the GP limit explained in the previous subsection.

One of the unresolved issues in the theory of superfluidity is its relation to Bose–Einstein condensation (BEC). It has been argued that in general neither condition is necessary for the other (c.f., e.g., [35, 2, 41]), but in the case considered here, i.e., the GP limit of a 3D gas, we show that 100% BEC into the constant wave function (in the rest frame) prevails even if an external velocity field is imposed. A simple example illustrating the fact that BEC is not necessary for superfluidity is the 1D hard-core Bose gas. This system is well known to have a spectrum like that of an ideal Fermi gas [24] (see also Sect. 8), and it is easy to see that it is superfluid in its ground state in the sense of (5.19). On the other hand, it has no BEC [43, 72]. The definition of the superfluid velocity as the gradient of the phase of the condensate wave function [34, 4] is clearly not applicable in such cases.

We consider a Bose gas with the Hamiltonian (2.1) in a box  $\mathcal{K}$  of side length  $L$ , assuming periodic boundary conditions in all three coordinate directions. Imposing an external velocity field  $\mathbf{v} = (0, 0, \pm|\mathbf{v}|)$  means that the momentum operator  $\mathbf{p} = -i\hbar\nabla$  is replaced by  $\mathbf{p} - m\mathbf{v}$ , retaining the periodic boundary conditions. The Hamiltonian in the moving frame is thus

$$H'_N = -\mu \sum_{j=1}^N \nabla_{j,\varphi}^2 + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|), \quad (5.20)$$

where  $\nabla_{j,\varphi} = \nabla_j + i(0, 0, \varphi/L)$  and the dimensionless phase  $\varphi$  is connected to the velocity  $\mathbf{v}$  by

$$\varphi = \frac{\pm|\mathbf{v}|Lm}{\hbar}. \quad (5.21)$$

Let  $E_0(N, a, \varphi)$  denote the ground state energy of (5.20) with periodic boundary conditions. Obviously it is no restriction to consider only the case  $-\pi \leq \varphi \leq \pi$ , since  $E_0$  is periodic in  $\varphi$  with period  $2\pi$  (see Remark 1 below). For  $\Psi_0$  the ground state of  $H'_N$ , let  $\gamma_N$  be its one-particle reduced density matrix. We are interested in the *Gross–Pitaevskii* (GP) limit  $N \rightarrow \infty$  with  $Na/L$  fixed. We also fix the box size  $L$ . This means that  $a$  should vary like  $1/N$  which, as explained in the previous subsection, can be achieved by writing  $v(r) = a^{-2}v_1(r/a)$ , where  $v_1$  is a fixed potential with scattering length 1, while  $a$  changes with  $N$ .

**Theorem 5.3 (Superfluidity and BEC of homogeneous gas).**

For  $|\varphi| \leq \pi$

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a, \varphi)}{N} = 4\pi\mu a\rho + \mu \frac{\varphi^2}{L^2} \quad (5.22)$$

in the limit  $N \rightarrow \infty$  with  $Na/L$  and  $L$  fixed. Here  $\rho = N/L^3$ , so  $a\rho$  is fixed too. In the same limit, for  $|\varphi| < \pi$ ,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \gamma_N(\mathbf{x}, \mathbf{x}') = \frac{1}{L^3} \quad (5.23)$$

in trace class norm, i.e.,  $\lim_{N \rightarrow \infty} \text{Tr} [ |\gamma_N/N - |L^{-3/2}\langle L^{-3/2} | | ] = 0$ .

Note that, by the definition (5.19) of  $\rho_s$  and (5.21), (5.22) means that  $\rho_s = \rho$ , i.e., there is 100% superfluidity. For  $\varphi = 0$ , (5.22) follows from (2.8), while (5.23) for  $\varphi = 0$  is the BEC of Theorem 5.1.<sup>3</sup>

*Remarks.* 1. By a unitary gauge transformation,

$$(U\Psi)(\mathbf{x}_1, \dots, \mathbf{x}_N) = e^{i\varphi(\sum_i z_i)/L} \Psi(\mathbf{x}_1, \dots, \mathbf{x}_N), \tag{5.24}$$

the passage from (2.1) to (5.20) is equivalent to replacing periodic boundary conditions in a box by the *twisted boundary condition*

$$\Psi(\mathbf{x}_1 + (0, 0, L), \mathbf{x}_2, \dots, \mathbf{x}_N) = e^{i\varphi} \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \tag{5.25}$$

in the direction of the velocity field, while retaining the original Hamiltonian (2.1).

2. The criterion  $|\varphi| \leq \pi$  means that  $|\mathbf{v}| \leq \pi\hbar/(mL)$ . The corresponding energy  $\frac{1}{2}m(\pi\hbar/(mL))^2$  is the gap in the excitation spectrum of the one-particle Hamiltonian in the finite-size system.

3. The reason that we have to restrict ourselves to  $|\varphi| < \pi$  in the second part of Theorem 5.3 is that for  $|\varphi| = \pi$  there are two ground states of the operator  $(\nabla + i\varphi/L)^2$  with periodic boundary conditions. All we can say in this case is that there is a subsequence of  $\gamma_N$  that converges to a density matrix of rank  $\leq 2$ , whose range is spanned by these two functions

*Proof (Theorem 5.3).* As in the proof of Theorem 5.1 we combine the localization Lemma 5.2, this time with  $\varphi \neq 0$ , and a generalized Poincaré inequality, this time Lemma 4.2. We thus infer that, for any symmetric  $\Psi$  with  $\langle \Psi, \Psi \rangle = 1$  and for  $N$  large enough,

$$\begin{aligned} & \frac{1}{N} \langle \Psi, H'_N \Psi \rangle (1 - \text{const. } Y^{1/17})^{-1} \\ & \geq 4\pi\mu\rho a + \mu \frac{\varphi^2}{L^2} - CY^{1/17} \left( \frac{1}{L^2} - \frac{1}{N} \langle \Psi, \sum_j \nabla_{j,\varphi}^2 \Psi \rangle \right) \\ & \quad + \frac{c}{L^2} \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} d\mathbf{x}_1 \left| \Psi(\mathbf{x}_1, \mathbf{X}) - L^{-3} \left[ \int_{\mathcal{K}} d\mathbf{x} \Psi(\mathbf{x}, \mathbf{X}) \right] \right|^2, \end{aligned} \tag{5.26}$$

where we used that  $|\Omega^c| \leq \frac{4\pi}{3}NR^3 = \text{const. } L^3Y^{2/17}$ . From this we can infer two things. First, since the kinetic energy, divided by  $N$ , is certainly bounded independently of  $N$ , as the upper bound shows, we get that

$$\liminf_{N \rightarrow \infty} \frac{E_0(N, a, \varphi)}{N} \geq 4\pi\mu\rho a + \mu \frac{\varphi^2}{L^2} \tag{5.27}$$

<sup>3</sup> The convention in Theorem 5.1, where  $\rho$  and  $Na/L$  stay fixed, is different from the one employed here, where  $L$  and  $Na/L$  are fixed, but these two conventions are clearly equivalent by scaling.



for any  $|\varphi| < \pi$ . By continuity this holds also for  $|\varphi| = \pi$ , proving (5.22). (To be precise,  $E_0/N - \mu\varphi^2 L^{-2}$  is concave in  $\varphi$ , and therefore stays concave, and in particular continuous, in the limit  $N \rightarrow \infty$ .) Secondly, since the upper and the lower bounds to  $E_0$  agree in the limit considered, the positive last term in (5.16) has to vanish in the limit. I.e., we get that for the ground state wave function  $\Psi_0$  of  $H'_N$

$$\lim_{N \rightarrow \infty} \int_{\mathcal{K}^{N-1}} d\mathbf{X} \int_{\mathcal{K}} dx_1 \left| \Psi_0(\mathbf{x}_1, \mathbf{X}) - L^{-3} \left[ \int_{\mathcal{K}} d\mathbf{x} \Psi_0(\mathbf{x}, \mathbf{X}) \right] \right|^2 = 0. \quad (5.28)$$

Using again (5.18), this proves (5.23) in a weak sense. As explained in [51, 52], this suffices for the convergence  $N^{-1}\gamma_N \rightarrow |L^{-3/2}\langle L^{-3/2} |$  in trace class norm.  $\square$

Theorem 5.3 can be generalized in various ways to a physically more realistic setting, for example replacing the periodic box by a cylinder centered at the origin. We shall comment on such extensions at the end of Sect. 7.

## 6 Gross–Pitaevskii Equation for Trapped Bosons

In the recent experiments on Bose condensation (see, e.g., [39]), 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  $V(\mathbf{x}) \rightarrow \infty$  as  $|\mathbf{x}| \rightarrow \infty$ . The Hamiltonian becomes

$$H = \sum_{i=1}^N \{-\mu\Delta_i + V(\mathbf{x}_i)\} + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|). \quad (6.1)$$

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

In the sequel we shall be considering a limit where  $a/L_{\text{osc}}$  tends to zero while  $N \rightarrow \infty$ . Experimentally  $a/L_{\text{osc}}$  can be changed in two ways: One can either vary  $L_{\text{osc}}$  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 [13]. Mathematically, both alternatives are equivalent, of course. The first corresponds to writing  $V(\mathbf{x}) = L_{\text{osc}}^{-2} V_1(\mathbf{x}/L_{\text{osc}})$  and keeping  $V_1$  and  $v$  fixed. The second corresponds to writing the interaction potential as  $v(|\mathbf{x}|) = a^{-2} v_1(|\mathbf{x}|/a)$  like in (5.4), 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 (6.1), measured in units of  $\hbar\omega$ , depends only on  $N$  and  $a/L_{\text{osc}}$ . In the dilute limit when  $a$  is much smaller than the mean particle distance, the energy becomes independent of  $v_1$ .

We choose  $L_{\text{osc}}$  as a length unit. The energy unit is  $\hbar\omega = 2\mu L_{\text{osc}}^{-2} = 2\mu$ . 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 (6.1) in an appropriate limit. This has been done in [53, 54] and in this section we give an account of this work. As we saw in Sects. 2 and 3 there is a difference in the  $\rho$  dependence between two and three dimensions, so we can expect a related difference now. We discuss 3D first.

### 6.1 Three Dimensions

Associated with the quantum mechanical ground state energy problem is the Gross–Pitaevskii (GP) energy functional [30, 31, 71]

$$\mathcal{E}^{\text{GP}}[\phi] = \int_{\mathbb{R}^3} (\mu|\nabla\phi|^2 + V|\phi|^2 + 4\pi\mu a|\phi|^4) \, \mathbf{d}\mathbf{x} \quad (6.2)$$

with the subsidiary condition

$$\int_{\mathbb{R}^3} |\phi|^2 = N. \quad (6.3)$$

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

$$E^{\text{GP}}(N, a) = \inf_{\int |\phi|^2 = N} \mathcal{E}^{\text{GP}}[\phi] = \mathcal{E}^{\text{GP}}[\phi^{\text{GP}}], \quad (6.4)$$

with a unique, positive  $\phi^{\text{GP}}$ . The existence of the minimizer  $\phi^{\text{GP}}$  is proved by standard techniques and it can be shown to be continuously differentiable, see [53], Sect. 2 and Appendix A. The minimizer depends on  $N$  and  $a$ , of course, and when this is important we denote it by  $\phi_{N,a}^{\text{GP}}$ .

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

$$-\mu\Delta\phi^{\text{GP}}(\mathbf{x}) + V(\mathbf{x})\phi^{\text{GP}}(\mathbf{x}) + 8\pi\mu a\phi^{\text{GP}}(\mathbf{x})^3 = \mu^{\text{GP}}\phi^{\text{GP}}(\mathbf{x}), \quad (6.5)$$

where  $\mu^{\text{GP}}$  is the chemical potential, given by

$$\mu^{\text{GP}} = \text{d}E^{\text{GP}}(N, a)/\text{d}N = E^{\text{GP}}(N, a)/N + (4\pi\mu a/N) \int |\phi^{\text{GP}}(\mathbf{x})|^4 \, \mathbf{d}\mathbf{x}. \quad (6.6)$$

The GP theory has the following scaling property:

$$E^{\text{GP}}(N, a) = N E^{\text{GP}}(1, Na), \quad (6.7)$$

and

$$\phi_{N,a}^{\text{GP}}(\mathbf{x}) = N^{1/2}\phi_{1,Na}^{\text{GP}}(\mathbf{x}). \quad (6.8)$$

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

We now turn to the relation of  $E^{\text{GP}}$  and  $\phi^{\text{GP}}$  to the quantum mechanical ground state. If  $v = 0$ , then the ground state of (6.1) is

$$\Psi_0(\mathbf{x}_1, \dots, \mathbf{x}_N) = \prod_{i=1}^N \phi_0(\mathbf{x}_i) \tag{6.9}$$

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

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

$$E_0 \approx E^{\text{GP}} \quad \text{and} \quad \rho^{\text{QM}}(\mathbf{x}) \approx |\phi^{\text{GP}}(\mathbf{x})|^2 \equiv \rho^{\text{GP}}(\mathbf{x}), \tag{6.10}$$

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

$$\rho^{\text{QM}}(\mathbf{x}) = N \int |\Psi_0(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N)|^2 d\mathbf{x}_2 \cdots d\mathbf{x}_N. \tag{6.11}$$

*Dilute* means here that

$$\bar{\rho} a^3 \ll 1, \tag{6.12}$$

where

$$\bar{\rho} = \frac{1}{N} \int |\rho^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x} \tag{6.13}$$

is the *mean density*.

The limit in which (6.10) can be expected to be true should be chosen so that *all three* terms in  $\mathcal{E}^{\text{GP}}$  make a contribution. The scaling relations (6.7) and (6.8) indicate that fixing  $Na$  as  $N \rightarrow \infty$  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  $10^4$  [14]). 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

$$a^3 \bar{\rho} \sim N^{-2}. \tag{6.14}$$

The precise statement of (6.10) is:

**Theorem 6.1 (GP limit of the QM ground state energy and density).**

*If  $N \rightarrow \infty$  with  $Na$  fixed, then*

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a)}{E^{\text{GP}}(N, a)} = 1, \tag{6.15}$$

and

$$\lim_{N \rightarrow \infty} \frac{1}{N} \rho_{N,a}^{\text{QM}}(\mathbf{x}) = |\phi_{1,Na}^{\text{GP}}(\mathbf{x})|^2 \tag{6.16}$$

*in the weak  $L^1$ -sense.*

Convergence can not only be proved for the ground state energy and density, but also for the individual energy components:

**Theorem 6.2 (Asymptotics of the energy components).** *Let  $\psi_0$  denote the solution to the zero-energy scattering equation for  $v$  (under the boundary condition  $\lim_{|\mathbf{x}|\rightarrow\infty} \psi_0(\mathbf{x}) = 1$ ) and  $s = \int |\nabla\psi_0|^2/(4\pi a)$ . Then  $0 < s \leq 1$  and, in the same limit as in Theorem 6.1 above,*

$$\begin{aligned} \lim_{N\rightarrow\infty} \int |\nabla_{\mathbf{x}_1}\Psi_0(\mathbf{x}_1, \mathbf{X})|^2 d\mathbf{x}_1 d\mathbf{X} \\ = \int |\nabla\phi_{1,Na}^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x} + 4\pi N a s \int |\phi_{1,Na}^{\text{GP}}(\mathbf{x})|^4 d\mathbf{x} , \end{aligned} \tag{6.17a}$$

$$\lim_{N\rightarrow\infty} \int V(\mathbf{x}_1)|\Psi_0(\mathbf{x}_1, \mathbf{X})|^2 d\mathbf{x}_1 d\mathbf{X} = \int V(\mathbf{x})|\phi_{1,Na}^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x} , \tag{6.17b}$$

$$\begin{aligned} \lim_{N\rightarrow\infty} \frac{1}{2} \sum_{j=2}^N \int v(|\mathbf{x}_1 - \mathbf{x}_j|)|\Psi_0(\mathbf{x}_1, \mathbf{X})|^2 d\mathbf{x}_1 d\mathbf{X} \\ = (1 - s)4\pi N a \int |\phi_{1,Na}^{\text{GP}}(\mathbf{x})|^4 d\mathbf{x} . \end{aligned} \tag{6.17c}$$

Here we introduced again the short hand notation (5.2). Theorem 6.2 is a simple consequence of Theorem 6.1 by variation with respect to the different components of the energy, as was also noted in [11]. More precisely, (6.15) can be written as

$$\lim_{N\rightarrow\infty} \frac{1}{N} E_0(N, a) = E^{\text{GP}}(1, Na) . \tag{6.18}$$

The ground state energy is a concave function of the mass parameter  $\mu$ , so it is legitimate to differentiate both sides of (6.18) with respect to  $\mu$ . In doing so, it has to be noted that  $Na$  depends on  $\mu$  through the scattering length. Using (2.13) one sees that

$$\frac{d(\mu a)}{d\mu} = \frac{1}{4\pi} \int |\nabla\psi_0|^2 d\mathbf{x} \tag{6.19}$$

by the Feynman–Hellmann principle, since  $\psi_0$  minimizes the left side of (2.13).

We remark that in the case of a two-dimensional Bose gas, where the relevant parameter to be kept fixed in the GP limit is  $N/|\ln(a^2\bar{\rho}_N)|$  (c.f. Sects. 3 and 6.2.), the parameter  $s$  in Theorem 6.2 can be shown to be always equal to 1. I.e., in 2D the interaction energy is purely kinetic in the GP limit (see [10]).

To describe situations where  $Na$  is very large, it is appropriate to consider a limit where, as  $N \rightarrow \infty$ ,  $a \gg N^{-1}$ , i.e.  $Na \rightarrow \infty$ , but still  $\bar{\rho}a^3 \rightarrow 0$ . 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*

$$\mathcal{E}^{\text{TF}}[\rho] = \int_{\mathbb{R}^3} (V\rho + 4\pi\mu a\rho^2) \, d\mathbf{x} \tag{6.20}$$

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  $\rho$  on  $\mathbb{R}^3$ . Its ground state energy  $E^{\text{TF}}$  and density  $\rho^{\text{TF}}$  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 Sect. 6.2 below).

Our second main result of this section is that minimization of (6.20) reproduces correctly the ground state energy and density of the many-body Hamiltonian in the limit when  $N \rightarrow \infty$ ,  $a^3\bar{\rho} \rightarrow 0$ , but  $Na \rightarrow \infty$  (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.,  $W(\lambda\mathbf{x}) = \lambda^s W(\mathbf{x})$  for all  $\lambda > 0$ , and locally Hölder continuous (see [54] for a precise definition). This condition can be relaxed, but it seems adequate for most practical applications and simplifies things considerably.

**Theorem 6.3 (TF limit of the QM ground state energy and density).**  
*Assume that  $V$  satisfies the conditions stated above. If  $g \equiv Na \rightarrow \infty$  as  $N \rightarrow \infty$ , but still  $a^3\bar{\rho} \rightarrow 0$ , then*

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a)}{E^{\text{TF}}(N, a)} = 1, \tag{6.21}$$

and

$$\lim_{N \rightarrow \infty} \frac{g^{3/(s+3)}}{N} \rho_{N,a}^{\text{QM}}(g^{1/(s+3)}\mathbf{x}) = \tilde{\rho}_{1,1}^{\text{TF}}(\mathbf{x}) \tag{6.22}$$

in the weak  $L^1$ -sense, where  $\tilde{\rho}_{1,1}^{\text{TF}}$  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 6.1 and 6.3. We will derive appropriate upper and lower bounds on the ground state energy  $E_0$ .

The proof of the lower bound in Theorem 6.1 presented here is a modified version of (and partly simpler than) the original proof in [53].

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 (Theorems 6.1 and 6.3). 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 [17], who used this function to give an upper bound on the ground state energy of the homogeneous hard core Bose gas (c.f. Sect. 2.1). It is of the form

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \prod_{i=1}^N \phi^{\text{GP}}(\mathbf{x}_i) F(\mathbf{x}_1, \dots, \mathbf{x}_N), \quad (6.23)$$

where  $F$  is constructed in the following way:

$$F(\mathbf{x}_1, \dots, \mathbf{x}_N) = \prod_{i=1}^N f(t_i(\mathbf{x}_1, \dots, \mathbf{x}_i)), \quad (6.24)$$

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

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } r < b, \\ 1 & \text{for } r \geq b, \end{cases} \quad (6.25)$$

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 (6.23) 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 [53] for details) is the upper bound

$$E_0(N, a) \leq E^{\text{GP}}(N, a) \left(1 + O(a\bar{\rho}^{1/3})\right). \quad (6.26)$$

*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  $\min_{\mathbf{x}} V(\mathbf{x})$  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  $\Psi$  as

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \prod_{i=1}^N \phi^{\text{GP}}(\mathbf{x}_i) F(\mathbf{x}_1, \dots, \mathbf{x}_N). \quad (6.27)$$

Here  $\phi^{\text{GP}} = \phi_{N,a}^{\text{GP}}$  is normalized so that  $\int |\phi^{\text{GP}}|^2 = N$ . Equation (6.27) defines  $F$  for a given  $\Psi$  because  $\phi^{\text{GP}}$  is everywhere strictly positive, being the ground

state of the operator  $-\Delta + V + 8\pi a|\phi^{\text{GP}}|^2$ . We now compute the expectation value of  $H$  in the state  $\Psi$ . Using partial integration and the variational equation (6.5) for  $\phi^{\text{GP}}$ , we see that

$$\frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle} - E^{\text{GP}}(N, a) = 4\pi a \int |\rho^{\text{GP}}|^2 + Q(F), \tag{6.28}$$

with

$$Q(F) = \frac{\sum_{i=1}^N \int \prod_{k=1}^N \rho^{\text{GP}}(\mathbf{x}_k) \left( |\nabla_i F|^2 + \left[ \frac{1}{2} \sum_{j \neq i} v(|\mathbf{x}_i - \mathbf{x}_j|) - 8\pi a \rho^{\text{GP}}(\mathbf{x}_i) \right] |F|^2 \right)}{\int \prod_{k=1}^N \rho^{\text{GP}}(\mathbf{x}_k) |F|^2}. \tag{6.29}$$

We recall that  $\rho^{\text{GP}}(\mathbf{x}) = |\phi_{N,a}^{\text{GP}}(\mathbf{x})|^2$ . 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  $\Psi$  itself we have thus obtained the replacements

$$V(\mathbf{x}) \rightarrow -8\pi a \rho^{\text{GP}}(\mathbf{x}) \quad \text{and} \quad \prod_{i=1}^N d\mathbf{x}_i \rightarrow \prod_{i=1}^N \rho^{\text{GP}}(\mathbf{x}_i) d\mathbf{x}_i. \tag{6.30}$$

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

$$\inf_F Q(F) \geq \inf_{\{n_\alpha\}} \sum_{\alpha} \inf_{F_\alpha} Q_\alpha(F_\alpha), \tag{6.31}$$

where  $Q_\alpha$  is defined by the same formula as  $Q$  but with the integrations limited to the box  $\alpha$ ,  $F_\alpha$  is a wave function with particle number  $n_\alpha$ , 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  $\infty$ , and restrict ourselves to boxes inside a cube  $\Lambda_M$  of side length  $M$ . Since  $v \geq 0$  the contribution to (6.31) of boxes outside this cube is easily estimated from below by  $-8\pi N a \sup_{\mathbf{x} \notin \Lambda_M} \rho^{\text{GP}}(\mathbf{x})$ , which, divided by  $N$ , is arbitrarily small for  $M$  large, since  $Na$  is fixed and  $\phi^{\text{GP}}/N^{1/2} = \phi_{1,Na}^{\text{GP}}$  decreases faster than exponentially at infinity ([53], Lemma A.5).

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

$$\Psi_\alpha(\mathbf{x}_1, \dots, \mathbf{x}_{n_\alpha}) = F_\alpha(\mathbf{x}_1, \dots, \mathbf{x}_{n_\alpha}) \prod_{k=1}^{n_\alpha} \phi^{\text{GP}}(\mathbf{x}_k), \tag{6.32}$$

and

$$\Psi_\alpha^{(i)}(\mathbf{x}_1, \dots, \mathbf{x}_{n_\alpha}) = F_\alpha(\mathbf{x}_1, \dots, \mathbf{x}_{n_\alpha}) \prod_{\substack{k=1 \\ k \neq i}}^{n_\alpha} \phi^{\text{GP}}(\mathbf{x}_k). \quad (6.33)$$

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

$$\begin{aligned} & \int \prod_{k=1}^{n_\alpha} \rho^{\text{GP}}(\mathbf{x}_k) (|\nabla_i F_\alpha|^2 + \frac{1}{2} \sum_{j \neq i} v(|\mathbf{x}_i - \mathbf{x}_j|) |F_\alpha|^2) \\ & \geq \rho_{\alpha, \min} \int (|\nabla_i \Psi_\alpha^{(i)}|^2 + \frac{1}{2} \sum_{j \neq i} v(|\mathbf{x}_i - \mathbf{x}_j|) |\Psi_\alpha^{(i)}|^2). \end{aligned} \quad (6.34)$$

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

$$(6.34) \geq \rho_{\alpha, \min} \int (\varepsilon |\nabla_i \Psi_\alpha^{(i)}|^2 + a(1 - \varepsilon) U(t_i) |\Psi_\alpha^{(i)}|^2) \quad (6.35)$$

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

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

$$|\nabla_i \Psi_\alpha|^2 \leq 2\rho_{\alpha, \max} |\nabla_i \Psi_\alpha^{(i)}|^2 + 2|\Psi_\alpha^{(i)}|^2 N C_M \quad (6.36)$$

with

$$C_M = \frac{1}{N} \sup_{\mathbf{x} \in \Lambda_M} |\nabla \phi^{\text{GP}}(\mathbf{x})|^2 = \sup_{\mathbf{x} \in \Lambda_M} |\nabla \phi_{1, Na}^{\text{GP}}(\mathbf{x})|^2. \quad (6.37)$$

Since  $Na$  is fixed,  $C_M$  is independent of  $N$ . Inserting (6.36) into (6.35), summing over  $i$  and using  $\rho^{\text{GP}}(\mathbf{x}_i) \leq \rho_{\alpha, \max}$  in the last term of (6.29) (in the box  $\alpha$ ), we get

$$Q_\alpha(F_\alpha) \geq \frac{\rho_{\alpha, \min}}{\rho_{\alpha, \max}} E_\varepsilon^U(n_\alpha, L) - 8\pi a \rho_{\alpha, \max} n_\alpha - \varepsilon C_M n_\alpha, \quad (6.38)$$

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

$$\sum_{i=1}^{n_\alpha} (-\frac{1}{2}\varepsilon \Delta_i + (1 - \varepsilon) a U(t_i)) \quad (6.39)$$

in the box (c.f. (2.35)). We want to minimize (6.38) with respect to  $n_\alpha$  and drop the subsidiary condition  $\sum_\alpha n_\alpha = N$  in (6.31). This can only lower the minimum. For the time being we also ignore the last term in (6.38). (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 (6.39), we can use the statement and proof of Theorem 2.4. From this we see that

$$E_\varepsilon^U(n_\alpha, L) \geq (1 - \varepsilon) \frac{4\pi a n_\alpha^2}{L^3} (1 - C Y_\alpha^{1/17}) \quad (6.40)$$



with  $Y_\alpha = a^3 n_\alpha / L^3$ , provided  $Y_\alpha$  is small enough,  $\varepsilon \geq Y_\alpha^{1/17}$  and  $n_\alpha \geq (\text{const.}) Y_\alpha^{-1/17}$ . The condition on  $\varepsilon$  is certainly fulfilled if we choose  $\varepsilon = Y^{1/17}$  with  $Y = a^3 N / L^3$ . We now want to show that the  $n_\alpha$  minimizing the right side of (6.38) is large enough for (6.40) to apply.

If the minimum of the right side of (6.38) (without the last term) is taken for some  $\bar{n}_\alpha$ , we have

$$\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} (E_\varepsilon^U(\bar{n}_\alpha + 1, L) - E_\varepsilon^U(\bar{n}_\alpha, L)) \geq 8\pi a \rho_{\alpha,\max} . \quad (6.41)$$

On the other hand, we claim that

**Lemma 6.4.** *For any  $n$*

$$E_\varepsilon^U(n + 1, L) - E_\varepsilon^U(n, L) \leq 8\pi a \frac{n}{L^3} . \quad (6.42)$$

*Proof.* Denote the operator (6.39) 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  $\mathbf{x}_i$  among the  $n + 1$  points  $\mathbf{x}_1, \dots, \mathbf{x}_{n+1}$  (without  $\mathbf{x}_i$ ) and  $t_i$  the corresponding distance excluding  $\mathbf{x}_{n+1}$ . Obviously, for  $1 \leq i \leq n$ ,

$$U(t'_i) \leq U(t_i) + U(|\mathbf{x}_i - \mathbf{x}_{n+1}|) \quad (6.43)$$

and

$$U(t'_{n+1}) \leq \sum_{i=1}^n U(|\mathbf{x}_i - \mathbf{x}_{n+1}|) . \quad (6.44)$$

Therefore

$$\tilde{H}_{n+1} \leq \tilde{H}_n - \frac{1}{2}\varepsilon \Delta_{n+1} + 2a \sum_{i=1}^n U(|\mathbf{x}_i - \mathbf{x}_{n+1}|) . \quad (6.45)$$

Using  $\tilde{\Psi}_n / L^{3/2}$  as trial function for  $\tilde{H}_{n+1}$  we arrive at (6.42). □

Equation (6.42) together with (6.41) 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 (6.40) 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  $Q_\alpha$  we therefore have to minimize

$$4\pi a \left( \frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \frac{n_\alpha^2}{L^3} \left( 1 - CY^{1/17} \right) - 2n_\alpha \rho_{\alpha,\max} \right) . \quad (6.46)$$

We can drop the requirement that  $n_\alpha$  has to be an integer. The minimum of (6.46) is obtained for

$$n_\alpha = \frac{\rho_{\alpha,\max}^2}{\rho_{\alpha,\min}} \frac{L^3}{(1 - CY^{1/17})} . \quad (6.47)$$

By (6.28) this gives the following lower bound, including now the last term in (6.38) as well as the contributions from the boxes outside  $\Lambda_M$ ,

$$\begin{aligned}
 & E_0(N, a) - E^{\text{GP}}(N, a) \\
 & \geq 4\pi a \int |\rho^{\text{GP}}|^2 - 4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha, \min}^2 L^3 \left( \frac{\rho_{\alpha, \max}^3}{\rho_{\alpha, \min}^3} \frac{1}{(1 - CY^{1/17})} \right) \\
 & \quad - Y^{1/17} N C_M - 4\pi a N \sup_{\mathbf{x} \notin \Lambda_M} \rho^{\text{GP}}(\mathbf{x}).
 \end{aligned} \tag{6.48}$$

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

$$\rho_{\alpha, \max} - \rho_{\alpha, \min} \leq N C' L, \quad \rho_{\alpha, \min} \geq N C'' . \tag{6.49}$$

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

$$\frac{\rho_{\alpha, \max}^3}{\rho_{\alpha, \min}^3} \frac{1}{(1 - CY^{1/17})} \leq 1 + (\text{const.}) N^{-1/10} \tag{6.50}$$

Also,

$$4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha, \min}^2 L^3 \leq 4\pi a \int |\rho^{\text{GP}}|^2 \leq E^{\text{GP}}(N, a) . \tag{6.51}$$

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

$$\frac{E_0(N, a)}{E^{\text{GP}}(N, a)} \geq 1 - (\text{const.})(1 + C_M) N^{-1/10} - (\text{const.}) \sup_{\mathbf{x} \notin \Lambda_M} |\phi_{1, Na}^{\text{GP}}|^2 , \tag{6.52}$$

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

*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  $Na \rightarrow \infty$ , 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

$$\rho_{N, a}^{\text{TF}}(\mathbf{x}) = \frac{1}{8\pi a} [\mu^{\text{TF}} - V(\mathbf{x})]_+ , \tag{6.53}$$

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

$$V(\mathbf{x}) \geq \mu^{\text{TF}} - 8\pi a \rho^{\text{TF}}(\mathbf{x}) \tag{6.54}$$

to get a replacement as in (6.30), but without changing the measure. Moreover,  $\rho^{\text{TF}}$  has compact support, so, applying again the box method described above, the boxes far out do not contribute to the energy. However,  $\mu^{\text{TF}}$  (which depends only on the combination  $Na$ ) tends to infinity as  $Na \rightarrow \infty$ . We

need to control the asymptotic behavior of  $\mu^{\text{TF}}$ , and this leads to the restrictions on  $V$  described in the paragraph preceding Theorem 6.3. For simplicity, we shall here only consider the case when  $V$  itself is homogeneous, i.e.,  $V(\lambda\mathbf{x}) = \lambda^s V(\mathbf{x})$  for all  $\lambda > 0$  with some  $s > 0$ .

In the same way as in (6.6) we have, with  $g = Na$ ,

$$\mu^{\text{TF}}(g) = dE^{\text{TF}}(N, a)/dN = E^{\text{TF}}(1, g) + 4\pi g \int |\rho_{1,g}^{\text{TF}}(\mathbf{x})|^2 d\mathbf{x}. \quad (6.55)$$

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

$$E^{\text{TF}}(1, g) = g^{s/(s+3)} E^{\text{TF}}(1, 1), \quad (6.56)$$

$$\mu^{\text{TF}}(g) = g^{s/(s+3)} \mu^{\text{TF}}(1), \quad (6.57)$$

and

$$g^{3/(s+3)} \rho_{1,g}^{\text{TF}}(g^{1/(s+3)}\mathbf{x}) = \rho_{1,g}^{\text{TF}}(\mathbf{x}). \quad (6.58)$$

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

$$\widehat{v}(\mathbf{x}) = g^{2/(s+3)} v(g^{1/(s+3)}\mathbf{x}) \quad (6.59)$$

with scattering length

$$\widehat{a} = g^{-1/(s+3)} a. \quad (6.60)$$

Using (6.54), (6.55) and the scaling relations we obtain

$$E_0(N, a) \geq E^{\text{TF}}(N, a) + 4\pi N g^{s/(s+3)} \int |\rho_{1,1}^{\text{TF}}|^2 + g^{-2/(s+3)} Q \quad (6.61)$$

with

$$Q = \inf_{\int |\Psi|^2 = 1} \sum_i \int (|\nabla_i \Psi|^2 + \frac{1}{2} \sum_{j \neq i} \widehat{v}(\mathbf{x}_i - \mathbf{x}_j) |\Psi|^2 - 8\pi N \widehat{a} \rho_{1,1}^{\text{TF}}(\mathbf{x}_i) |\Psi|^2). \quad (6.62)$$

We can now proceed exactly as in Part 2 to arrive at the analogy of (6.48), which in the present case becomes

$$E_0(N, a) - E^{\text{TF}}(N, a) \geq 4\pi N g^{s/(s+3)} \int |\rho_{1,1}^{\text{TF}}|^2 - 4\pi N \widehat{a} \sum_{\alpha} \rho_{\alpha, \max}^2 L^3 (1 - C \widehat{Y}^{1/17})^{-1}. \quad (6.63)$$

Here  $\rho_{\alpha, \max}$  is the maximum of  $\rho_{1,1}^{\text{TF}}$  in the box  $\alpha$ , 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

$$\bar{\rho} = N \bar{\rho}_{1,g} \sim N g^{-3/(s+3)} \bar{\rho}_{1,1}, \quad (6.64)$$

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

$$\liminf_{N \rightarrow \infty} \frac{E_0(N, a)}{E^{\text{TF}}(N, a)} \geq 1 \quad (6.65)$$

in the limit  $N \rightarrow \infty$ ,  $a^3 \bar{\rho} \rightarrow 0$ . Here we used the fact that (because  $V$ , and hence  $\rho^{\text{TF}}$ , is continuous by assumption) the Riemann sum  $\sum_{\alpha} \rho_{\alpha, \max}^2 L^3$  converges to  $\int |\rho_{1,1}^{\text{TF}}|^2$  as  $L \rightarrow 0$ . Together with the upper bound (6.26) and the fact that  $E^{\text{GP}}(N, a)/E^{\text{TF}}(N, a) = E^{\text{GP}}(1, Na)/E^{\text{TF}}(1, Na) \rightarrow 1$  as  $Na \rightarrow \infty$ , which holds under our regularity assumption on  $V$  (c.f. Lemma 2.3 in [54]), this proves (6.15) and (6.21).

*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

$$V(\mathbf{x}) \longrightarrow V(\mathbf{x}) + \delta g^{s/(s+3)} Z(g^{-1/(s+3)} \mathbf{x}) \quad (6.66)$$

for some positive  $Z \in C_0^\infty$  and redoing the upper and lower bounds we see that (6.21) holds with  $W$  replaced by  $W + \delta Z$ . Differentiating with respect to  $\delta$  at  $\delta = 0$  yields

$$\lim_{N \rightarrow \infty} \frac{g^{3/(s+3)}}{N} \rho_{N,a}^{\text{QM}}(g^{1/(s+3)} \mathbf{x}) = \tilde{\rho}_{1,1}^{\text{TF}}(\mathbf{x}) \quad (6.67)$$

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.  $\square$

## 6.2 Two Dimensions

In contrast to the three-dimensional case the energy per particle for a dilute gas in two dimensions is *nonlinear* in  $\rho$ . 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

$$4\pi \int_{\mathbb{R}^2} |\ln(|\phi(\mathbf{x})|^2 a^2)|^{-1} |\phi(\mathbf{x})|^4 d\mathbf{x}, \quad (6.68)$$

and such a term has, indeed, been suggested in [80] and [40]. 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)

$$\mathcal{E}^{\text{GP}}[\phi] = \int_{\mathbb{R}^2} (|\nabla\phi|^2 + V|\phi|^2 + 4\pi\alpha|\phi|^4) \, d\mathbf{x} , \quad (6.69)$$

where instead of  $a$  the coupling constant is now

$$\alpha = |\ln(\bar{\rho}_N a^2)|^{-1} \quad (6.70)$$

with  $\bar{\rho}_N$  the *mean density* for the GP functional at coupling constant 1 and particle number  $N$ . This is defined analogously to (6.13) as

$$\bar{\rho}_N = \frac{1}{N} \int |\phi_{N,1}^{\text{GP}}|^4 \, d\mathbf{x} \quad (6.71)$$

where  $\phi_{N,1}^{\text{GP}}$  is the minimizer of (6.69) with  $\alpha = 1$  and subsidiary condition  $\int |\phi|^2 = N$ . Note that  $\alpha$  in (6.70) depends on  $N$  through the mean density.

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

$$E^{\text{GP}}(N, \alpha) = N E^{\text{GP}}(1, N\alpha) \quad (6.72)$$

and

$$N^{-1/2} \phi_{N,\alpha}^{\text{GP}} = \phi_{1,N\alpha}^{\text{GP}} , \quad (6.73)$$

hold, and the relevant parameter is

$$g \equiv N\alpha . \quad (6.74)$$

In three dimensions, where  $\alpha = a$ , it is natural to consider the limit  $N \rightarrow \infty$  with  $g = Na = \text{const}$ . The analogue of Theorem 6.1 in two dimensions is

**Theorem 6.5 (Two-dimensional GP limit theorem).** *If, for  $N \rightarrow \infty$ ,  $a^2 \bar{\rho}_N \rightarrow 0$  with  $g = N/|\ln(a^2 \bar{\rho}_N)|$  fixed, then*

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a)}{E^{\text{GP}}(N, 1/|\ln(a^2 \bar{\rho}_N)|)} = 1 \quad (6.75)$$

and

$$\lim_{N \rightarrow \infty} \frac{1}{N} \rho_{N,a}^{\text{QM}}(\mathbf{x}) = |\phi_{1,g}^{\text{GP}}(\mathbf{x})|^2 \quad (6.76)$$

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  $N \rightarrow \infty$  and  $g \rightarrow \infty$  (but still  $\bar{\rho}_N a^2 \rightarrow 0$ ).

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

$$V(\lambda \mathbf{x}) = \lambda^s V(\mathbf{x}) \tag{6.77}$$

for some  $s > 0$ , this limit can be described by the ‘Thomas–Fermi’ energy functional like (6.20) with coupling constant unity:

$$\mathcal{E}^{\text{TF}}[\rho] = \int_{\mathbb{R}^2} (V(\mathbf{x})\rho(\mathbf{x}) + 4\pi\rho(\mathbf{x})^2) \, d\mathbf{x} . \tag{6.78}$$

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

$$\int \rho(\mathbf{x})d\mathbf{x} = 1 . \tag{6.79}$$

The minimizer of (6.78) can be given explicitly. It is

$$\rho_{1,1}^{\text{TF}}(\mathbf{x}) = (8\pi)^{-1}[\mu^{\text{TF}} - V(\mathbf{x})]_+ \tag{6.80}$$

where the chemical potential  $\mu^{\text{TF}}$  is determined by the normalization condition (6.79) and  $[t]_+ = t$  for  $t \geq 0$  and zero otherwise. We denote the corresponding energy by  $E^{\text{TF}}(1, 1)$ . By scaling one obtains

$$\lim_{g \rightarrow \infty} E^{\text{GP}}(1, g)/g^{s/(s+2)} = E^{\text{TF}}(1, 1) , \tag{6.81}$$

$$\lim_{g \rightarrow \infty} g^{2/(s+2)} \rho_{1,g}^{\text{GP}}(g^{1/(s+2)} \mathbf{x}) = \rho_{1,1}^{\text{TF}}(\mathbf{x}) , \tag{6.82}$$

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

Our main result about two-dimensional Bose gases in external potentials satisfying (6.77) is that analogous limits also hold for the many-particle quantum mechanical ground state at low densities:

**Theorem 6.6 (Two-dimensional TF limit theorem).** *In two dimensions, if  $a^2 \bar{\rho}_N \rightarrow 0$ , but  $g = N/|\ln(\bar{\rho}_N a^2)| \rightarrow \infty$  as  $N \rightarrow \infty$  then*

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a)}{g^{s/s+2}} = E^{\text{TF}}(1, 1) \tag{6.83}$$

and, in the weak  $L^1$  sense,

$$\lim_{N \rightarrow \infty} \frac{g^{2/(s+2)}}{N} \rho_{N,a}^{\text{QM}}(g^{1/(s+2)} \mathbf{x}) = \rho_{1,1}^{\text{TF}}(\mathbf{x}) . \tag{6.84}$$

*Remarks.* 1. As in Theorem 6.3, it is sufficient that  $V$  is asymptotically equal to some homogeneous potential,  $W$ . In this case,  $E^{\text{TF}}(1, 1)$  and  $\rho_{1,1}^{\text{TF}}$  in Theorem 6.6 should be replaced by the corresponding quantities for  $W$ .

2. From (6.82) it follows that

$$\bar{\rho}_N \sim N^{s/(s+2)} \tag{6.85}$$

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

We shall now comment briefly on the proofs of Theorems 6.5 and 6.6, 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 6.5 the point to notice is that the expression (6.46), that has to be minimized over  $n_\alpha$ , is in 2D replaced by

$$4\pi \left( \frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \frac{n_\alpha^2}{L^2} \frac{1}{|\ln(a^2 n_\alpha / L^2)|} \left( 1 - \frac{C}{|\ln(a^2 N / L^2)|^{1/5}} \right) - \frac{2n_\alpha \rho_{\alpha,\max}}{|\ln(a^2 \bar{\rho}_N)|} \right), \tag{6.86}$$

since (6.40) has to be replaced by the analogous inequality for 2D (c.f. (3.31)). To minimize (6.86) we use the following lemma:

**Lemma 6.7.** *For  $0 < x, b < 1$  and  $k \geq 1$  we have*

$$\frac{x^2}{|\ln x|} - 2 \frac{b}{|\ln b|} x k \geq - \frac{b^2}{|\ln b|} \left( 1 + \frac{1}{(2|\ln b|)^2} \right) k^2. \tag{6.87}$$

*Proof.* Replacing  $x$  by  $xk$  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

$$\frac{x^2}{b^2} \frac{|\ln b|}{|\ln x|} - 2 \frac{x}{b} \geq \frac{|\ln b|}{b^2} e d x^{2+d} - \frac{2x}{b} \geq c(d) (b^d e d |\ln b|)^{-1/(1+d)} \tag{6.88}$$

with

$$c(d) = 2^{(2+d)/(1+d)} \left( \frac{1}{(2+d)^{(2+d)/(1+d)}} - \frac{1}{(2+d)^{1/(1+d)}} \right) \geq -1 - \frac{1}{4} d^2. \tag{6.89}$$

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

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

$$k = \frac{\rho_{\alpha,\max}}{\rho_{\alpha,\min}} \left( 1 - \frac{C}{|\ln(a^2 N / L^2)|^{1/5}} \right)^{-1} \frac{|\ln(a^2 \rho_{\alpha,\max})|}{|\ln(a^2 \bar{\rho}_N)|} \tag{6.90}$$

we get the bound

$$(6.86) \geq -4\pi \frac{\rho_{\alpha,\max}^2 L^2}{|\ln(a^2 \bar{\rho}_N)|} \left( 1 + \frac{1}{4|\ln(a^2 \rho_{\alpha,\max})|^2} \right) k. \tag{6.91}$$

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

The TF case, Thm. 6.6, 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.

## 7 Bose–Einstein Condensation and Superfluidity for Dilute Trapped Gases

It was shown in the previous section 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 5.1 and although it is not the same as BEC in the thermodynamic limit it is quite relevant for the actual experiments with Bose gases in traps. In the following, we concentrate on the 3D case, but analogous considerations apply also to the 2D case. We also discuss briefly some extensions of Theorem 5.3 pertaining to superfluidity in trapped gases.

As in the last section we choose to keep the length scale  $L_{\text{osc}}$  of the confining potential fixed and thus write  $Na$  instead of  $Na/L_{\text{osc}}$ . Consequently the powers of  $N$  appearing in the proofs are different from those in the proof Theorem 5.1, where we kept  $Na/L$  and  $N/L^3$  fixed.

For use later, we define the projector

$$P^{\text{GP}} = |\phi^{\text{GP}}\rangle\langle\phi^{\text{GP}}|. \quad (7.1)$$

Here (and everywhere else in this section) we denote  $\phi^{\text{GP}} \equiv \phi_{1,Na}^{\text{GP}}$  for simplicity, where  $\phi_{1,Na}^{\text{GP}}$  is the minimizer of the GP functional (6.2) with parameter  $Na$  and normalization condition  $\int |\phi|^2 = 1$  (compare with (6.8)). Moreover, we set  $\mu \equiv 1$ .

In the following,  $\Psi_0$  denotes the (nonnegative and normalized) ground state of the Hamiltonian (6.1). BEC refers to the reduced one-particle density matrix  $\gamma(\mathbf{x}, \mathbf{x}')$  of  $\Psi_0$ , defined in (5.1). The precise definition of BEC is that for some  $c > 0$  this integral operator has for all large  $N$  an eigenfunction with eigenvalue  $\geq cN$ .

Complete (or 100%) BEC is defined to be the property that  $\frac{1}{N}\gamma(\mathbf{x}, \mathbf{x}')$  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,  $\frac{1}{N}\gamma(\mathbf{x}, \mathbf{x}')$  becomes a simple product  $\varphi(\mathbf{x})^*\varphi(\mathbf{x}')$  as  $N \rightarrow \infty$ , in which case  $\varphi$  is called the *condensate wave function*. In the GP limit, i.e.,  $N \rightarrow \infty$  with  $Na$  fixed, we can show that this is the case, and the condensate wave function is, in fact, the GP minimizer  $\phi^{\text{GP}}$ .

### Theorem 7.1 (Bose–Einstein condensation in a trap).

For each fixed  $Na$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \gamma(\mathbf{x}, \mathbf{x}') = \phi^{\text{GP}}(\mathbf{x})\phi^{\text{GP}}(\mathbf{x}') \quad (7.2)$$

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



We remark that Theorem 7.1 implies that there is also 100% condensation for all  $n$ -particle reduced density matrices

$$\begin{aligned} &\gamma^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{x}'_1, \dots, \mathbf{x}'_n) = \\ &n! \binom{N}{n} \int \Psi_0(\mathbf{x}_1, \dots, \mathbf{x}_N) \Psi_0(\mathbf{x}'_1, \dots, \mathbf{x}'_n, \mathbf{x}_{n+1}, \dots, \mathbf{x}_N) d\mathbf{x}_{n+1} \cdots d\mathbf{x}_N \end{aligned} \quad (7.3)$$

of  $\Psi_0$ , i.e., they converge, after division by the normalization factor, to the one-dimensional projector onto the  $n$ -fold tensor product of  $\phi^{\text{GP}}$ . In other words, for  $n$  fixed particles the probability of finding them all in the same state  $\phi^{\text{GP}}$  tends to 1 in the limit considered. To see this, let  $a^*, a$  denote the boson creation and annihilation operators for the state  $\phi^{\text{GP}}$ , and observe that

$$1 \geq \lim_{N \rightarrow \infty} N^{-n} \langle \Psi_0 | (a^*)^n a^n | \Psi_0 \rangle = \lim_{N \rightarrow \infty} N^{-n} \langle \Psi_0 | (a^* a)^n | \Psi_0 \rangle, \quad (7.4)$$

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

$$N^{-n} \langle \Psi_0 | (a^* a)^n | \Psi_0 \rangle \geq N^{-n} \langle \Psi_0 | a^* a | \Psi_0 \rangle^n, \quad (7.5)$$

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

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

**Corollary 7.2 (Convergence of momentum distribution).** *Let*

$$\widehat{\rho}(\mathbf{k}) = \int \int \gamma(\mathbf{x}, \mathbf{x}') \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] d\mathbf{x} d\mathbf{x}' \quad (7.6)$$

*denote the one-particle momentum density of  $\Psi_0$ . Then, for fixed  $Na$ ,*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \widehat{\rho}(\mathbf{k}) = |\widehat{\phi}^{\text{GP}}(\mathbf{k})|^2 \quad (7.7)$$

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

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

$$\begin{aligned} \left| \frac{1}{N} \int \widehat{\rho} h - \int |\widehat{\phi}^{\text{GP}}|^2 h \right| &= |\text{Tr} [\mathcal{F}^{-1}(\gamma/N - P^{\text{GP}}) \mathcal{F} h]| \\ &\leq \|h\|_\infty \text{Tr} |\gamma/N - P^{\text{GP}}|, \end{aligned} \quad (7.8)$$

from which we conclude that

$$\|\widehat{\rho}/N - |\widehat{\phi}^{\text{GP}}|^2\|_1 \leq \text{Tr} |\gamma/N - P^{\text{GP}}|. \quad (7.9)$$

□

As already stated, Theorem 7.1 is a generalization of Theorem 5.1, 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 5.1 the box size grows as  $N^{1/3}$  to keep the density fixed, while in Theorem 7.1 we choose to keep the confining external potential fixed. Both conventions are equivalent, of course, c.f. the remarks in the second paragraph of Sect. 6, but when comparing the exponents of  $N$  that appear in the proofs of the two theorems the different conventions should be born in mind.

As in Theorem 5.1 there are two essential components of our proof of Theorem 7.1. The first is a proof that the part of the kinetic energy that is associated with the interaction  $v$  (namely, the second term in (6.17a)) 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  $N^{-1/3}$ . (The exponents differ from those of Lemma 5.2 because of different scaling conventions.) This allows us to conclude that the function of  $\mathbf{x}$  defined for each fixed value of  $\mathbf{X}$  by

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{\phi^{\text{GP}}(\mathbf{x})} \psi_0(\mathbf{x}, \mathbf{X}) \geq 0 \quad (7.10)$$

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

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  $\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})$  in this set does not guarantee that  $f_{\mathbf{X}}(\mathbf{x})$  is nearly constant (in  $\mathbf{x}$ ), or even that it is continuous. We need  $f_{\mathbf{X}}(\mathbf{x})$  to be nearly constant in order to conclude BEC. What saves the day is the knowledge that the total kinetic energy of  $f_{\mathbf{X}}(\mathbf{x})$  (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  $f_{\mathbf{X}}(\mathbf{x})$  is the generalized Poincaré inequality in Lemma 4.3. The important point in this lemma is that there is no restriction on  $\Omega$  concerning regularity or connectivity.

Using the results of Theorem 6.2, partial integration and the GP equation (i.e., the variational equation for  $\phi^{\text{GP}}$ , see (6.5)) we see that

$$\lim_{N \rightarrow \infty} \int |\phi^{\text{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 d\mathbf{x} d\mathbf{X} = 4\pi N a s \int |\phi^{\text{GP}}(\mathbf{x})|^4 d\mathbf{x}. \quad (7.11)$$

The following Lemma shows that to leading order all the energy in (7.11) is concentrated in small balls.

**Lemma 7.3 (Localization of the energy in a trap).** *For fixed  $\mathbf{X}$  let*

$$\Omega_{\mathbf{X}} = \left\{ \mathbf{x} \in \mathbb{R}^3 \mid \min_{k \geq 2} |\mathbf{x} - \mathbf{x}_k| \geq N^{-1/3-\delta} \right\} \quad (7.12)$$

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

$$\lim_{N \rightarrow \infty} \int d\mathbf{X} \int_{\Omega_{\mathbf{x}}} d\mathbf{x} |\phi^{\text{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 = 0. \quad (7.13)$$

*Remark.* In the proof of Theorem 5.1 we chose  $\delta$  to be  $4/51$ , but the following proof shows that one can extend the range of  $\delta$  beyond this value.

*Proof.* We shall show that

$$\begin{aligned} & \int d\mathbf{X} \int_{\Omega_{\mathbf{x}}} d\mathbf{x} |\phi^{\text{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2 \\ & + \int d\mathbf{X} \int d\mathbf{x} |\phi^{\text{GP}}(\mathbf{x})|^2 |f_{\mathbf{X}}(\mathbf{x})|^2 \left[ \frac{1}{2} \sum_{k \geq 2} v(|\mathbf{x} - \mathbf{x}_k|) - 8\pi Na |\phi^{\text{GP}}(\mathbf{x})|^2 \right] \\ & \geq -4\pi Na \int |\phi^{\text{GP}}(\mathbf{x})|^4 d\mathbf{x} - o(1) \end{aligned} \quad (7.14)$$

as  $N \rightarrow \infty$ . We claim that this implies the assertion of the Lemma. To see this, note that the left side of (7.14) can be written as

$$\frac{1}{N} E_0 - \mu^{\text{GP}} - \int d\mathbf{X} \int_{\Omega_{\mathbf{x}}} d\mathbf{x} |\phi^{\text{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{X}}(\mathbf{x})|^2, \quad (7.15)$$

where we used partial integration and the GP equation (6.5), and also the symmetry of  $\Psi_0$ . The convergence of the energy in Theorem 6.1 and the relation (6.6) now imply the desired result.

The proof of (7.14) is actually just a detailed examination of the lower bounds to the energy derived in [53] and [62] and described in Sects. 2 and 6. We use the same methods as there, just describing the differences from the case considered here.

Writing

$$f_{\mathbf{X}}(\mathbf{x}) = \prod_{k \geq 2} \phi^{\text{GP}}(\mathbf{x}_k) F(\mathbf{x}, \mathbf{X}) \quad (7.16)$$

and using that  $F$  is symmetric in the particle coordinates, we see that (7.14) is equivalent to

$$\frac{1}{N} Q_{\delta}(F) \geq -4\pi Na \int |\phi^{\text{GP}}|^4 - o(1), \quad (7.17)$$

where  $Q_{\delta}$  is the quadratic form

$$\begin{aligned} Q_{\delta}(F) &= \sum_{i=1}^N \int_{\Omega_i^c} |\nabla_i F|^2 \prod_{k=1}^N |\phi^{\text{GP}}(\mathbf{x}_k)|^2 d\mathbf{x}_k \\ &+ \sum_{1 \leq i < j \leq N} \int v(|\mathbf{x}_i - \mathbf{x}_j|) |F|^2 \prod_{k=1}^N |\phi^{\text{GP}}(\mathbf{x}_k)|^2 d\mathbf{x}_k \\ &- 8\pi Na \sum_{i=1}^N \int |\phi^{\text{GP}}(\mathbf{x}_i)|^2 |F|^2 \prod_{k=1}^N |\phi^{\text{GP}}(\mathbf{x}_k)|^2 d\mathbf{x}_k. \end{aligned} \quad (7.18)$$

Here  $\Omega_i^c$  denotes the set

$$\Omega_i^c = \{(\mathbf{x}_1, \mathbf{X}) \in \mathbb{R}^{3N} \mid \min_{k \neq i} |\mathbf{x}_i - \mathbf{x}_k| \leq N^{-1/3-\delta}\} . \tag{7.19}$$

While (7.17) is not true for all conceivable  $F$ 's satisfying the normalization condition

$$\int |F(\mathbf{x}, \mathbf{X})|^2 \prod_{k=1}^N |\phi^{\text{GP}}(\mathbf{x}_k)|^2 d\mathbf{x}_k = 1 , \tag{7.20}$$

it *is* true for an  $F$ , such as ours, that has bounded kinetic energy (7.11). Looking at Sect. 6, we see that (6.28)–(6.29), (6.48)–(6.52) are similar to (7.17), (7.18) and almost establish (7.17), 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  $\min_{k \neq i} |\mathbf{x}_i - \mathbf{x}_k| \leq N^{-1/3-\delta}$ . However, looking at the proof of the lower bound to the ground state energy of a homogeneous Bose gas discussed in Sect. 2, which enters the proof of Theorem 6.1, 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 (7.11).) We can even do better and choose some  $4/51 < \delta < 2/9$ , if  $\alpha$  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  $\alpha$  small enough). The choice of  $\alpha$  only affects the magnitude of the error term, however, which is still  $o(1)$  as  $N \rightarrow \infty$ . □

*Proof (Theorem 7.1).* For some  $R > 0$  let  $\mathcal{K} = \{\mathbf{x} \in \mathbb{R}^3, |\mathbf{x}| \leq R\}$ , and define

$$\langle f_{\mathbf{x}} \rangle_{\mathcal{K}} = \frac{1}{\int_{\mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x}} \int_{\mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 f_{\mathbf{x}}(\mathbf{x}) d\mathbf{x} . \tag{7.21}$$

We shall use Lemma 4.3, with  $d = 3$ ,  $h(\mathbf{x}) = |\phi^{\text{GP}}(\mathbf{x})|^2 / \int_{\mathcal{K}} |\phi^{\text{GP}}|^2$ ,  $\Omega = \Omega_{\mathbf{x}} \cap \mathcal{K}$  and  $f(\mathbf{x}) = f_{\mathbf{x}}(\mathbf{x}) - \langle f_{\mathbf{x}} \rangle_{\mathcal{K}}$  (see (7.12) and (7.10)). Since  $\phi^{\text{GP}}$  is bounded on  $\mathcal{K}$  above and below by some positive constants, this Lemma also holds (with a different constant  $C'$ ) with  $d\mathbf{x}$  replaced by  $|\phi^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x}$  in (4.6). Therefore,

$$\begin{aligned} & \int d\mathbf{X} \int_{\mathcal{K}} d\mathbf{x} |\phi^{\text{GP}}(\mathbf{x})|^2 [f_{\mathbf{x}}(\mathbf{x}) - \langle f_{\mathbf{x}} \rangle_{\mathcal{K}}]^2 \\ & \leq C' \int d\mathbf{X} \left[ \int_{\Omega_{\mathbf{x}} \cap \mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{x}}(\mathbf{x})|^2 d\mathbf{x} \right. \\ & \quad \left. + \frac{N^{-2\delta}}{R^2} \int_{\mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 |\nabla_{\mathbf{x}} f_{\mathbf{x}}(\mathbf{x})|^2 d\mathbf{x} \right] , \end{aligned} \tag{7.22}$$

where we used that  $|\Omega_{\mathbf{x}}^c \cap \mathcal{K}| \leq (4\pi/3)N^{-3\delta}$ . The first integral on the right side of (7.22) tends to zero as  $N \rightarrow \infty$  by Lemma 7.3, and the second is bounded by (7.11). We conclude, since

$$\int_{\mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \leq \int_{\mathbb{R}^3} |\phi^{\text{GP}}(\mathbf{x})|^2 f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \tag{7.23}$$

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

$$\begin{aligned} \liminf_{N \rightarrow \infty} \frac{1}{N} \langle \phi^{\text{GP}} | \gamma | \phi^{\text{GP}} \rangle &\geq \int_{\mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x} \lim_{N \rightarrow \infty} \int d\mathbf{X} \int_{\mathcal{K}} d\mathbf{x} |\Psi_0(\mathbf{x}, \mathbf{X})|^2 \\ &= \left[ \int_{\mathcal{K}} |\phi^{\text{GP}}(\mathbf{x})|^2 d\mathbf{x} \right]^2, \end{aligned} \tag{7.24}$$

where the last equality follows from (6.16). Since the radius of  $\mathcal{K}$  was arbitrary, we conclude that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \langle \phi^{\text{GP}} | \gamma | \phi^{\text{GP}} \rangle = 1, \tag{7.25}$$

implying convergence of  $\gamma/N$  to  $P^{\text{GP}}$  in Hilbert–Schmidt norm. Since the traces are equal, convergence even holds in trace norm (cf. [81], Thm. 2.20), and Theorem 7.1 is proven.  $\square$

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 [54, 63], c.f. Sects. 3 and 6.2. 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 [33, 66]. In the hard core lattice gas at half filling precisely this phenomenon occurs [38].

Finally, we remark on generalizations of Theorem 5.3 on superfluidity from a torus to some physically more realistic settings. As an example, let  $\mathcal{C}$  be a finite cylinder based on an annulus centered at the origin. Given a bounded, real function  $a(r, z)$  let  $A$  be the vector field (in polar coordinates)  $A(r, \theta, z) = \varphi a(r, z) \hat{e}_\theta$ , where  $\hat{e}_\theta$  is the unit vector in the  $\theta$  direction. We also allow for a bounded external potential  $V(r, z)$  that does not depend on  $\theta$ .

Using the methods of Appendix A in [53], it is not difficult to see that there exists a  $\varphi_0 > 0$ , depending only on  $\mathcal{C}$  and  $a(r, z)$ , such that for all  $|\varphi| < \varphi_0$  there is a unique minimizer  $\phi^{\text{GP}}$  of the Gross–Pitaevskii functional

$$\mathcal{E}^{\text{GP}}[\phi] = \int_{\mathcal{C}} \left( |(\nabla + iA(\mathbf{x}))\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + 4\pi\mu Na|\phi(\mathbf{x})|^4 \right) d\mathbf{x} \tag{7.26}$$

under the normalization condition  $\int |\phi|^2 = 1$ . This minimizer does not depend on  $\theta$ , and can be chosen to be positive, for the following reason: The relevant term in the kinetic energy is  $T = -r^{-2}[\partial/\partial\theta + i\varphi r a(r, z)]^2$ . If  $|\varphi r a(r, z)| < 1/2$ , it is easy to see that  $T \geq \varphi^2 a(r, z)^2$ , in which case, without raising the energy, we can replace  $\phi$  by the square root of the  $\theta$ -average of  $|\phi|^2$ . This can only lower the kinetic energy [49] and, by convexity of  $x \rightarrow x^2$ , this also lowers the  $\phi^4$  term.

We denote the ground state energy of  $\mathcal{E}^{\text{GP}}$  by  $E^{\text{GP}}$ , depending on  $Na$  and  $\varphi$ . The following Theorem 7.4 concerns the ground state energy  $E_0$  of

$$H_N^A = \sum_{j=1}^N \left[ -(\nabla_j + iA(\mathbf{x}_j))^2 + V(\mathbf{x}_j) \right] + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|), \quad (7.27)$$

with Neumann boundary conditions on  $\mathcal{C}$ , and the one-particle reduced density matrix  $\gamma_N$  of the ground state, respectively. Different boundary conditions can be treated in the same manner, if they are also used in (7.26).

*Remark.* As a special case, consider a uniformly rotating system. In this case  $A(\mathbf{x}) = \varphi r \widehat{e}_\theta$ , where  $2\varphi$  is the angular velocity.  $H_N^A$  is the Hamiltonian in the rotating frame, but with external potential  $V(\mathbf{x}) + A(\mathbf{x})^2$  (see e.g. [4, p. 131]).

**Theorem 7.4 (Superfluidity in a cylinder).** For  $|\varphi| < \varphi_0$

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a, \varphi)}{N} = E^{\text{GP}}(Na, \varphi) \quad (7.28)$$

in the limit  $N \rightarrow \infty$  with  $Na$  fixed. In the same limit,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \gamma_N(\mathbf{x}, \mathbf{x}') = \phi^{\text{GP}}(\mathbf{x}) \phi^{\text{GP}}(\mathbf{x}') \quad (7.29)$$

in trace class norm, i.e.,  $\lim_{N \rightarrow \infty} \text{Tr} [ |\gamma_N/N - |\phi^{\text{GP}}\rangle\langle\phi^{\text{GP}}| | ] = 0$ .

In the case of a uniformly rotating system, where  $2\varphi$  is the angular velocity, the condition  $|\varphi| < \varphi_0$  in particular means that the angular velocity is smaller than the critical velocity for creating vortices [79, 21].

*Remark.* In the special case of the curl-free vector potential  $A(r, \theta) = \varphi r^{-1} \widehat{e}_\theta$ , i.e.,  $a(r, z) = r^{-1}$ , one can say more about the role of  $\varphi_0$ . In this case, there is a unique GP minimizer for all  $\varphi \notin \mathbb{Z} + \frac{1}{2}$ , whereas there are two minimizers for  $\varphi \in \mathbb{Z} + \frac{1}{2}$ . Part two of Theorem 7.4 holds in this special case for all  $\varphi \notin \mathbb{Z} + \frac{1}{2}$ , and (7.28) is true even for all  $\varphi$ .

## 8 One-Dimensional Behavior of Dilute Bose Gases in Traps

Recently it has become possible to do experiments in highly elongated traps on ultra-cold Bose gases that are effectively one-dimensional [8, 27, 29, 76, 65]. These experiments show peculiar features predicted by a model of a one-dimensional Bose gas with repulsive  $\delta$ -function pair interaction, analyzed long ago by Lieb and Liniger [48]. These include quasi-fermionic behavior [24], the absence of Bose–Einstein condensation (BEC) in a dilute limit [43, 72, 26], and an excitation spectrum different from that predicted by Bogoliubov’s

theory [48, 37, 42]. The theoretical work on the dimensional cross-over for the ground state in elongated traps has so far been based either on variational calculations, starting from a 3D delta-potential [67, 15, 25], or on numerical Quantum Monte Carlo studies [6, 1] with more realistic, genuine 3D potentials, but particle numbers limited to the order of 100. This work is important and has led to valuable insights, in particular about different parameter regions [70, 16], but a more thorough theoretical understanding is clearly desirable since this is not a simple problem. In fact, it is evident that for a potential with a hard core the true 3D wave functions do not approximately factorize in the longitudinal and transverse variables (otherwise the energy would be infinite) and the effective 1D potential can not be obtained by simply integrating out the transverse variables of the 3D potential (that would immediately create an impenetrable barrier in 1D). It is important to be able to demonstrate rigorously, and therefore unambiguously, that the 1D behavior really follows from the fundamental Schrödinger equation. It is also important to delineate, as we do here, precisely what can be seen in the different parameter regions. The full proofs of our assertions are long and are given in [58]. Here we state our main results and outline the basic ideas for the proofs.

We start by describing the setting more precisely. It is convenient to write the Hamiltonian in the following way (in units where  $\hbar = 2m = 1$ ):

$$H_{N,L,r,a} = \sum_{j=1}^N (-\Delta_j + V_r^\perp(\mathbf{x}_j^\perp) + V_L(z_j)) + \sum_{1 \leq i < j \leq N} v_a(|\mathbf{x}_i - \mathbf{x}_j|) \quad (8.1)$$

with  $\mathbf{x} = (x, y, z) = (\mathbf{x}^\perp, z)$  and with

$$\begin{aligned} V_r^\perp(\mathbf{x}^\perp) &= \frac{1}{r^2} V^\perp(\mathbf{x}^\perp/r), \\ V_L(z) &= \frac{1}{L^2} V(z/L), \quad v_a(|\mathbf{x}|) = \frac{1}{a^2} v(|\mathbf{x}|/a). \end{aligned} \quad (8.2)$$

Here,  $r, L, a$  are variable scaling parameters while  $V^\perp, V$  and  $v$  are fixed.

We shall be concerned with the ground state of this Hamiltonian for large particle number  $N$ , which is appropriate for the consideration of actual experiments. The other parameters of the problem are the scattering length,  $a$ , of the two-body interaction potential,  $v$ , and two lengths,  $r$  and  $L$ , describing the transverse and the longitudinal extension of the trap potential, respectively.

The interaction potential  $v$  is supposed to be nonnegative, of finite range and have scattering length 1; the scaled potential  $v_a$  then has scattering length  $a$ . The external trap potentials  $V$  and  $V^\perp$  confine the motion in the longitudinal ( $z$ ) and the transversal ( $\mathbf{x}^\perp$ ) directions, respectively, and are assumed to be continuous and tend to  $\infty$  as  $|z|$  and  $|\mathbf{x}^\perp|$  tend to  $\infty$ . To simplify the discussion we find it also convenient to assume that  $V$  is homogeneous of some order  $s > 0$ , namely  $V(z) = |z|^s$ , but weaker assumptions, e.g. asymptotic homogeneity (cf. Sect. 6), would in fact suffice. The case of a simple box with

hard walls is realized by taking  $s = \infty$ , while the usual harmonic approximation is  $s = 2$ . It is understood that the lengths associated with the ground states of  $-\mathrm{d}^2/\mathrm{d}z^2 + V(z)$  and  $-\Delta^\perp + V^\perp(\mathbf{x}^\perp)$  are both of the order 1 so that  $L$  and  $r$  measure, respectively, the longitudinal and the transverse extensions of the trap. We denote the ground state energy of (8.1) by  $E^{\mathrm{QM}}(N, L, r, a)$  and the ground state particle density by  $\rho_{N,L,r,a}^{\mathrm{QM}}(\mathbf{x})$ . On the average, this 3D density will always be low in the parameter range considered here (in the sense that distance between particles is large compared to the 3D scattering length). The effective 1D density can be either high or low, however.

In parallel with the 3D Hamiltonian we consider the Hamiltonian for  $n$  Bosons in 1D with delta interaction and coupling constant  $g \geq 0$ , i.e.,

$$H_{n,g}^{\mathrm{1D}} = \sum_{j=1}^n -\partial^2/\partial z_j^2 + g \sum_{1 \leq i < j \leq n} \delta(z_i - z_j). \quad (8.3)$$

We consider this Hamiltonian for the  $z_j$  in an interval of length  $\ell$  in the thermodynamic limit,  $\ell \rightarrow \infty$ ,  $n \rightarrow \infty$  with  $\rho = n/\ell$  fixed. The ground state energy per particle in this limit is independent of boundary conditions and can, according to [48], be written as

$$e_0^{\mathrm{1D}}(\rho) = \rho^2 e(g/\rho), \quad (8.4)$$

with a function  $e(t)$  determined by a certain integral equation. Its asymptotic form is  $e(t) \approx \frac{1}{2}t$  for  $t \ll 1$  and  $e(t) \rightarrow \pi^2/3$  for  $t \rightarrow \infty$ . Thus

$$e_0^{\mathrm{1D}}(\rho) \approx \frac{1}{2}g\rho \quad \text{for } g/\rho \ll 1 \quad (8.5)$$

and

$$e_0^{\mathrm{1D}}(\rho) \approx (\pi^2/3)\rho^2 \quad \text{for } g/\rho \gg 1. \quad (8.6)$$

This latter energy is the same as for non-interacting fermions in 1D, which can be understood from the fact that (8.3) with  $g = \infty$  is equivalent to a Hamiltonian describing free fermions.

Taking  $\rho e_0^{\mathrm{1D}}(\rho)$  as a local energy density for an inhomogeneous 1D system we can form the energy functional

$$\mathcal{E}[\rho] = \int_{-\infty}^{\infty} (|\nabla\sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z))) \mathrm{d}z. \quad (8.7)$$

Its ground state energy is obtained by minimizing over all normalized densities, i.e.,

$$E^{\mathrm{1D}}(N, L, g) = \inf \left\{ \mathcal{E}[\rho] : \rho(z) \geq 0, \int_{-\infty}^{\infty} \rho(z) \mathrm{d}z = N \right\}. \quad (8.8)$$

Using convexity of the map  $\rho \mapsto \rho^3 e(g/\rho)$ , it is standard to show that there exists a unique minimizer of (8.7) (see, e.g., [53]). It will be denoted by  $\rho_{N,L,g}$ . We also define the *mean 1D density* of this minimizer to be



$$\bar{\rho} = \frac{1}{N} \int_{-\infty}^{\infty} (\rho_{N,L,g}(z))^2 dz . \tag{8.9}$$

In a rigid box, i.e., for  $s = \infty$ ,  $\bar{\rho}$  is simply  $N/L$  (except for boundary corrections), but in more general traps it depends also on  $g$  besides  $N$  and  $L$ . The order of magnitude of  $\bar{\rho}$  in the various parameter regions will be described below.

Our main result relates the 3D ground state energy of (8.1) to the 1D density functional energy  $E^{1D}(N, L, g)$  in the large  $N$  limit with  $g \sim a/r^2$  provided  $r/L$  and  $a/r$  are sufficiently small. To state this precisely, let  $e^\perp$  and  $b(\mathbf{x}^\perp)$ , respectively, denote the ground state energy and the normalized ground state wave function of  $-\Delta^\perp + V^\perp(\mathbf{x}^\perp)$ . The corresponding quantities for  $-\Delta^\perp + V_r^\perp(\mathbf{x}^\perp)$  are  $e^\perp/r^2$  and  $b_r(\mathbf{x}^\perp) = (1/r)b(\mathbf{x}^\perp/r)$ . In the case that the trap is a cylinder with hard walls  $b$  is a Bessel function; for a quadratic  $V^\perp$  it is a Gaussian.

Define  $g$  by

$$g = \frac{8\pi a}{r^2} \int |b(\mathbf{x}^\perp)|^4 d\mathbf{x}^\perp = 8\pi a \int |b_r(\mathbf{x}^\perp)|^4 d\mathbf{x}^\perp . \tag{8.10}$$

Our main result of this section is:

**Theorem 8.1 (From 3D to 1D).** *Let  $N \rightarrow \infty$  and simultaneously  $r/L \rightarrow 0$  and  $a/r \rightarrow 0$  in such a way that  $r^2\bar{\rho} \times \min\{\bar{\rho}, g\} \rightarrow 0$ . Then*

$$\lim \frac{E^{\text{QM}}(N, L, r, a) - Ne^\perp/r^2}{E^{1D}(N, L, g)} = 1 . \tag{8.11}$$

An analogous result hold for the ground state density. Define the 1D QM density by averaging over the transverse variables, i.e.,

$$\hat{\rho}_{N,L,r,a}^{\text{QM}}(z) \equiv \int \rho_{N,L,r,a}^{\text{QM}}(\mathbf{x}^\perp, z) d\mathbf{x}^\perp . \tag{8.12}$$

Let  $\bar{L} := N/\bar{\rho}$  denote the extension of the system in  $z$ -direction, and define the rescaled density  $\tilde{\rho}$  by

$$\rho_{N,L,g}^{1D}(z) = \frac{N}{\bar{L}} \tilde{\rho}(z/\bar{L}) . \tag{8.13}$$

Note that, although  $\tilde{\rho}$  depends on  $N, L$  and  $g$ ,  $\|\tilde{\rho}\|_1 = \|\tilde{\rho}\|_2 = 1$ , which shows in particular that  $\bar{L}$  is the relevant scale in  $z$ -direction. The result for the ground state density is:

**Theorem 8.2 (1D limit for density).** *In the same limit as considered in Theorem 8.1,*

$$\lim \left( \frac{\bar{L}}{N} \hat{\rho}_{N,L,r,a}^{\text{QM}}(z\bar{L}) - \tilde{\rho}(z) \right) = 0 \tag{8.14}$$

*in weak  $L^1$  sense.*

Note that because of (8.5) and (8.6) the condition  $r^2\bar{\rho} \times \min\{\bar{\rho}, g\} \rightarrow 0$  is the same as

$$e_0^{1D}(\bar{\rho}) \ll 1/r^2, \quad (8.15)$$

i.e., the average energy per particle associated with the longitudinal motion should be much smaller than the energy gap between the ground and first excited state of the confining Hamiltonian in the transverse directions. Thus, the basic physics is highly quantum-mechanical and has no classical counterpart. The system can be described by a 1D functional (8.7), *even though the transverse trap dimension is much larger than the range of the atomic forces.*

## 8.1 Discussion of the Results

We will now give a discussion of the various parameter regions that are included in the limit considered in Theorems 8.1 and 8.2 above. We begin by describing the division of the space of parameters into two basic regions. This decomposition will eventually be refined into five regions, but for the moment let us concentrate on the basic dichotomy.

In Sect. 6 we proved that the 3D Gross–Pitaevskii formula for the energy is correct to leading order in situations in which  $N$  is large but  $a$  is small compared to the mean particle distance. This energy has two parts: The energy necessary to confine the particles in the trap, plus the internal energy of interaction, which is  $N4\pi a\rho^{3D}$ . This formula was proved to be correct for a *fixed* confining potential in the limit  $N \rightarrow \infty$  with  $a^3\rho^{3D} \rightarrow 0$ . However, this limit does not hold uniformly if  $r/L$  gets small as  $N$  gets large. In other words, new physics can come into play as  $r/L \rightarrow 0$  and it turns out that this depends on the ratio of  $a/r^2$  to the 1D density, or, in other words, on  $g/\bar{\rho}$ . There are two basic regimes to consider in highly elongated traps, i.e., when  $r \ll L$ . They are

- The 1D limit of the 3D Gross–Pitaevskii regime
- The ‘true’ 1D regime.

The former is characterized by  $g/\bar{\rho} \ll 1$ , while in the latter regime  $g/\bar{\rho}$  is of the order one or even tends to infinity. (If  $g/\bar{\rho} \rightarrow \infty$  the particles are effectively impenetrable; this is usually referred to as the Girardeau–Tonks region.) These two situations correspond to high 1D density (weak interaction) and low 1D density (strong interaction), respectively. Physically, the main difference is that in the strong interaction regime the motion of the particles in the longitudinal direction is highly correlated, while in the weak interaction regime it is not. Mathematically, this distinction also shows up in our proofs. The first region is correctly described by both the 3D and 1D theories because the two give the same predictions there. That’s why we call the second region the ‘true’ 1D regime.

In both regions the internal energy of the gas is small compared to the energy of confinement. However, this in itself does not imply a specifically

1D behavior. (If  $a$  is sufficiently small it is satisfied in a trap of any shape.) 1D behavior, when it occurs, manifests itself by the fact that the transverse motion of the atoms is uncorrelated while the longitudinal motion is correlated (very roughly speaking) in the same way as pearls on a necklace. Thus, the true criterion for 1D behavior is that  $g/\bar{\rho}$  is of order unity or larger and not merely the condition that the energy of confinement dominates the internal energy.

We shall now briefly describe the finer division of these two regimes into five regions altogether. Three of them (Regions 1–3) belong to the weak interaction regime and two (Regions 4–5) to the strong interaction regime. They are characterized by the behavior of  $g/\bar{\rho}$  as  $N \rightarrow \infty$ . In each of these regions the general functional (8.7) can be replaced by a different, simpler functional, and the energy  $E^{1D}(N, L, g)$  in Theorem 8.1 by the ground state energy of that functional. Analogously, the density in Theorem 8.2 can be replaced by the minimizer of the functional corresponding to the region considered.

The five regions are

- **Region 1, the Ideal Gas case:** In the trivial case where the interaction is so weak that it effectively vanishes in the large  $N$  limit and everything collapses to the ground state of  $-\frac{d^2}{dz^2} + V(z)$  with ground state energy  $e^{\parallel}$ , the energy  $E^{1D}$  in (8.11) can be replaced by  $Ne^{\parallel}/L^2$ . This is the case if  $g/\bar{\rho} \ll N^{-2}$ , and the mean density is just  $\bar{\rho} \sim N/L$ . Note that  $g/\bar{\rho} \ll N^{-2}$  means that the 3D interaction energy per particle  $\sim a\rho^{3D} \ll 1/L^2$ .

- **Region 2, the 1D GP case:** In this region  $g/\bar{\rho} \sim N^{-2}$ , with  $\bar{\rho} \sim N/L$ . This case is described by a 1D Gross–Pitaevskii energy functional of the form

$$\mathcal{E}^{\text{GP}}[\rho] = \int_{-\infty}^{\infty} (|\nabla\sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \frac{1}{2}g\rho(z)^2) dz, \quad (8.16)$$

corresponding to the high density approximation (8.5) of the interaction energy in (8.7). Its ground state energy,  $E^{\text{GP}}$ , fulfills the scaling relation  $E^{\text{GP}}(N, L, g) = NL^{-2}E^{\text{GP}}(1, 1, NgL)$ .

- **Region 3, the 1D TF case:**  $N^{-2} \ll g/\bar{\rho} \ll 1$ , with  $\bar{\rho}$  being of the order  $\bar{\rho} \sim (N/L)(NgL)^{-1/(s+1)}$ , where  $s$  is the degree of homogeneity of the longitudinal confining potential  $V$ . This region is described by a Thomas–Fermi type functional

$$\mathcal{E}^{\text{TF}}[\rho] = \int_{-\infty}^{\infty} (V_L(z)\rho(z) + \frac{1}{2}g\rho(z)^2) dz. \quad (8.17)$$

It is a limiting case of Region 2 in the sense that  $NgL \gg 1$ , but  $a/r$  is sufficiently small so that  $g/\bar{\rho} \ll 1$ , i.e., the high density approximation in (8.5) is still valid. The explanation of the factor  $(NgL)^{1/(s+1)}$  is as follows: The linear extension  $\bar{L}$  of the minimizing density of (8.16) is for large values of  $NgL$  determined by  $V_L(\bar{L}) \sim g(N/\bar{L})$ , which gives  $\bar{L} \sim (NgL)^{1/(s+1)}L$ . In addition condition (8.15) requires  $g\bar{\rho} \ll r^{-2}$ , which means that  $Na/L(NgL)^{1/(s+1)} \ll$

1. The minimum energy of (8.17) has the scaling property  $E^{\text{TF}}(N, L, g) = NL^{-2}(NgL)^{s/(s+1)}E^{\text{TF}}(1, 1, 1)$ .

• **Region 4, the LL case:**  $g/\bar{\rho} \sim 1$ , with  $\bar{\rho} \sim (N/L)N^{-2/(s+2)}$ , described by an energy functional

$$\mathcal{E}^{\text{LL}}[\rho] = \int_{-\infty}^{\infty} (V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z))) dz. \quad (8.18)$$

This region corresponds to the case  $g/\bar{\rho} \sim 1$ , so that neither the high density (8.5) nor the low density approximation (8.6) is valid and the full LL energy (8.4) has to be used. The extension  $\bar{L}$  of the system is now determined by  $V_L(\bar{L}) \sim (N/\bar{L})^2$  which leads to  $\bar{L} \sim LN^{2/(s+2)}$ . Condition (8.15) means in this region that  $Nr/\bar{L} \sim N^{s/(s+2)}r/L \rightarrow 0$ . Since  $Nr/\bar{L} \sim (\bar{\rho}/g)(a/r)$ , this condition is automatically fulfilled if  $g/\bar{\rho}$  is bounded away from zero and  $a/r \rightarrow 0$ . The ground state energy of (8.18),  $E^{\text{LL}}(N, L, g)$ , is equal to  $N\gamma^2 E^{\text{LL}}(1, 1, g/\gamma)$ , where we introduced the density parameter  $\gamma := (N/L)N^{-2/(s+2)}$ .

• **Region 5, the GT case:**  $g/\bar{\rho} \gg 1$ , with  $\bar{\rho} \sim (N/L)N^{-2/(s+2)}$ , described by a functional with energy density  $\sim \rho^3$ , corresponding to the Girardeau–Tonks limit of the LL energy density. It corresponds to impenetrable particles, i.e., the limiting case  $g/\bar{\rho} \rightarrow \infty$  and hence formula (8.6) for the energy density. As in Region 4, the mean density is here  $\bar{\rho} \sim \gamma$ . The energy functional is

$$\mathcal{E}^{\text{GT}}[\rho] = \int_{-\infty}^{\infty} (V_L(z)\rho(z) + (\pi^2/3)\rho(z)^3) dz, \quad (8.19)$$

with minimum energy  $E^{\text{GT}}(N, L) = N\gamma^2 E^{\text{GT}}(1, 1)$ .

As already mentioned above, Regions 1–3 can be reached as limiting cases of a 3D Gross–Pitaevskii theory. In this sense, the behavior in these regions contains remnants of the 3D theory, which also shows up in the fact that BEC prevails in Regions 1 and 2 (See [58] for details.) Heuristically, these traces of 3D can be understood from the fact that in Regions 1–3 the 1D formula for energy per particle,  $g\rho \sim aN/(r^2L)$ , gives the same result as the 3D formula, i.e., scattering length times 3D density. This is no longer so in Regions 4 and 5 and different methods are required.

## 8.2 Outline of Proof

We now outline the main steps in the proof of Theorems 8.1 and 8.2, referring to [58] for full details. To prove (8.11) one has to establish upper and lower bounds, with controlled errors, on the QM many-body energy in terms of the energies obtained by minimizing the energy functionals appropriate for the various regions. The limit theorem for the densities can be derived from the energy estimates in a standard way by variation with respect to the external potential  $V_L$ .

The different parameter regions have to be treated by different methods, a watershed lying between Regions 1–3 on the one hand and Regions 4–5 on the other. In Regions 1–3, similar methods as in the proof of the 3D Gross–Pitaevskii limit theorem discussed in Sect. 6 can be used. This 3D proof needs some modifications, however, because there the external potential was fixed and the estimates are not uniform in the ratio  $r/L$ . We will not go into the details here, but mainly focus on Regions 4 and 5, where new methods are needed. It turns out to be necessary to localize the particles by dividing the trap into finite ‘boxes’ (finite in  $z$ -direction), with a controllable particle number in each box. The particles are then distributed optimally among the boxes to minimize the energy, in a similar way as (2.52) was derived from (2.47).

A core lemma for Regions 4–5 is an estimate of the 3D ground state energy in a finite box in terms of the 1D energy of the Hamiltonian (8.3). I.e., we will consider the ground state energy of (8.1) with the external potential  $V_L(z)$  replaced by a finite box (in  $z$ -direction) with length  $\ell$ . Let  $E_D^{QM}(n, \ell, r, a)$  and  $E_N^{QM}(n, \ell, r, a)$  denote its ground state energy with Dirichlet and Neumann boundary conditions, respectively.

**Lemma 8.3.** *Let  $E_D^{1D}(n, \ell, g)$  and  $E_N^{1D}(n, \ell, g)$  denote the ground state energy of (8.3) on  $L^2([0, \ell]^n)$ , with Dirichlet and Neumann boundary conditions, respectively, and let  $g$  be given by (8.10). Then there is a finite number  $C > 0$  such that*

$$E_N^{QM}(n, \ell, r, a) - \frac{ne^\perp}{r^2} \geq E_N^{1D}(n, \ell, g) \times \left( 1 - Cn \left( \frac{a}{r} \right)^{1/8} \left[ 1 + \frac{nr}{\ell} \left( \frac{a}{r} \right)^{1/8} \right] \right). \tag{8.20}$$

Moreover,

$$E_D^{QM}(n, \ell, r, a) - \frac{ne^\perp}{r^2} \leq E_D^{1D}(n, \ell, g) \times \left( 1 + C \left[ \left( \frac{na}{r} \right)^2 \left( 1 + \frac{al}{r^2} \right) \right]^{1/3} \right), \tag{8.21}$$

provided the term in square brackets is less than 1.

This Lemma is the key to the proof of Theorems 8.1 and 8.2. The reader interested in the details is referred to [58]. Here we only give a sketch of the proof of Lemma 8.3.

*Proof (Lemma 8.3).* We start with the upper bound (8.21). Let  $\psi$  denote the ground state of (8.3) with Dirichlet boundary conditions, normalized by  $\langle \psi | \psi \rangle = 1$ , and let  $\rho_\psi^{(2)}$  denote its two-particle density, normalized by  $\int \rho_\psi^{(2)}(z, z') dz dz' = 1$ . Let  $G$  and  $F$  be given by  $G(\mathbf{x}_1, \dots, \mathbf{x}_n) =$

$\psi(z_1, \dots, z_n) \prod_{j=1}^n b_r(\mathbf{x}_j^\perp)$  and  $F(\mathbf{x}_1, \dots, \mathbf{x}_n) = \prod_{i < j} f(|\mathbf{x}_i - \mathbf{x}_j|)$ . Here  $f$  is a monotone increasing function, with  $0 \leq f \leq 1$  and  $f(t) = 1$  for  $t \geq R$  for some  $R \geq R_0$ . For  $t \leq R$  we shall choose  $f(t) = f_0(t)/f_0(R)$ , where  $f_0$  is the solution to the zero-energy scattering equation for  $v_a$  (2.3). Note that  $f_0(R) = 1 - a/R$  for  $R \geq R_0$ , and  $f'_0(t) \leq t^{-1} \min\{1, a/t\}$ . We use as a trial wave function

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_n) = G(\mathbf{x}_1, \dots, \mathbf{x}_n)F(\mathbf{x}_1, \dots, \mathbf{x}_n). \tag{8.22}$$

We first have to estimate the norm of  $\Psi$ . Using the fact that  $F$  is 1 whenever no pair of particles is closer together than a distance  $R$ , we obtain

$$\langle \Psi | \Psi \rangle \geq 1 - \frac{n(n-1)}{2} \frac{\pi R^2}{r^2} \|b\|_4^4. \tag{8.23}$$

To evaluate the expectation value of the Hamiltonian, we use

$$\langle \Psi | -\Delta_j | \Psi \rangle = - \int F^2 G \Delta_j G + \int G^2 |\nabla_j F|^2 \tag{8.24}$$

and the Schrödinger equation  $H_{n,g}\psi = E_D^{1D}\psi$ . This gives

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= \left( E_D^{1D} + \frac{n}{r^2} e^\perp \right) \langle \Psi | \Psi \rangle - g \langle \Psi | \sum_{i < j} \delta(z_i - z_j) | \Psi \rangle \\ &+ \int G^2 \left( \sum_{j=1}^n |\nabla_j F|^2 + \sum_{i < j} v_a(|\mathbf{x}_i - \mathbf{x}_j|) |F|^2 \right). \end{aligned} \tag{8.25}$$

Now, since  $0 \leq f \leq 1$  and  $f' \geq 0$  by assumption,  $F^2 \leq f(|\mathbf{x}_i - \mathbf{x}_j|)^2$ , and

$$\sum_{j=1}^n |\nabla_j F|^2 \leq 2 \sum_{i < j} f'(|\mathbf{x}_i - \mathbf{x}_j|)^2 + 4 \sum_{k < i < j} f'(|\mathbf{x}_k - \mathbf{x}_i|) f'(|\mathbf{x}_k - \mathbf{x}_j|). \tag{8.26}$$

Consider the first term on the right side of (8.26), together with the last term in (8.25). These terms are bounded above by

$$n(n-1) \int b_r(\mathbf{x}^\perp)^2 b_r(\mathbf{y}^\perp)^2 \rho_\psi^{(2)}(z, z') (f'(|\mathbf{x} - \mathbf{y}|)^2 + \frac{1}{2} v_a(|\mathbf{x} - \mathbf{y}|) f(|\mathbf{x} - \mathbf{y}|)^2). \tag{8.27}$$

Let

$$h(z) = \int (f'(|\mathbf{x}|)^2 + \frac{1}{2} v_a(|\mathbf{x}|) f(|\mathbf{x}|)^2) d\mathbf{x}^\perp. \tag{8.28}$$

Using Young's inequality for the integration over the  $\perp$ -variables, we get

$$(8.27) \leq \frac{n(n-1)}{r^2} \|b\|_4^4 \int_{\mathbb{R}^2} \rho_\psi^{(2)}(z, z') h(z - z') dz dz'. \tag{8.29}$$

By similar methods, one can show that the contribution from the last term in (8.26) is bounded by

$$\frac{2}{3}n(n-1)(n-2)\frac{\|b\|_\infty^2}{r^2}\frac{\|b\|_4^4}{r^2}\|k\|_\infty\int_{\mathbb{R}^2}\rho_\psi^{(2)}(z,z')k(z-z')dzdz', \quad (8.30)$$

where

$$k(z) = \int f'(|\mathbf{x}|)d\mathbf{x}^\perp. \quad (8.31)$$

Note that both  $h$  and  $k$  are supported in  $[-R, R]$ .

Now, for any  $\phi \in H^1(\mathbb{R})$ ,

$$|\phi(z)|^2 - |\phi(z')|^2 \leq 2|z - z'|^{1/2} \left( \int_{\mathbb{R}} |\phi|^2 \right)^{1/4} \left( \int_{\mathbb{R}} \left| \frac{d\phi}{dz} \right|^2 \right)^{3/4}. \quad (8.32)$$

Applying this to  $\rho_\psi^{(2)}(z, z')$ , considered as a function of  $z$  only, we get

$$\begin{aligned} \int_{\mathbb{R}^2} \rho_\psi^{(2)}(z, z')h(z - z')dzdz' - \int_{\mathbb{R}} h(z)dz \int \rho_\psi^{(2)}(z, z)dz \\ \leq 2R^{1/2} \int_{\mathbb{R}} h(z)dz \left\langle \psi \left| -\frac{d^2}{dz^2} \right| \psi \right\rangle^{3/4}, \end{aligned} \quad (8.33)$$

where we used Schwarz's inequality, the normalization of  $\rho_\psi^{(2)}$  and the symmetry of  $\psi$ . The same argument is used for (8.30) with  $h$  replaced by  $k$ .

It remains to bound the second term in (8.25). As in the estimate for the norm of  $\Psi$ , we use again the fact that  $F$  is equal to 1 as long as the particles are not within a distance  $R$ . We obtain

$$\langle \Psi | \sum_{i < j} \delta(z_i - z_j) | \Psi \rangle \geq \frac{n(n-1)}{2} \int \rho_\psi^{(2)}(z, z)dz \left( 1 - \frac{n(n-1)}{2} \frac{\pi R^2}{r^2} \|b\|_4^4 \right). \quad (8.34)$$

We also estimate  $g\frac{1}{2}n(n-1) \int \rho_\psi^{(2)}(z, z)dz \leq E_D^{1D}$  and  $\langle \psi | -d^2/dz^2 | \psi \rangle \leq E_D^{1D}/n$ . We have  $\int h(z)dz = 4\pi a(1 - a/R)^{-1}$ , and the terms containing  $k$  can be bounded by  $\|k\|_\infty \leq 2\pi a(1 + \ln(R/a))/(1 - a/r)$  and  $\int k(z)dz \leq 2\pi aR(1 - a/(2R))/(1 - a/r)$ . Putting together all the bounds, and choosing

$$R^3 = \frac{ar^2}{n^2(1 + g\ell)}, \quad (8.35)$$

this proves the desired result.

We are left with the lower bound (8.20). We write a general wave function  $\Psi$  as

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_n) = f(\mathbf{x}_1, \dots, \mathbf{x}_n) \prod_{k=1}^n b_r(\mathbf{x}_k^\perp), \quad (8.36)$$

which can always be done, since  $b_r$  is a strictly positive function. Partial integration gives

$$\langle \Psi | H | \Psi \rangle = \frac{ne^\perp}{r^2} + \sum_{i=1}^n \int \left[ |\nabla_i f|^2 + \frac{1}{2} \sum_{j, j \neq i} v_a(|\mathbf{x}_i - \mathbf{x}_j|) |f|^2 \right] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k. \quad (8.37)$$

Choose some  $R > R_0$ , fix  $i$  and  $\mathbf{x}_j$ ,  $j \neq i$ , and consider the Voronoi cell  $\Omega_j$  around particle  $j$ , i.e.,  $\Omega_j = \{\mathbf{x} : |\mathbf{x} - \mathbf{x}_j| \leq |\mathbf{x} - \mathbf{x}_k| \text{ for all } k \neq j\}$ . If  $\mathcal{B}_j$  denotes the ball of radius  $R$  around  $\mathbf{x}_j$ , we can estimate with the aid of Lemma 2.5

$$\begin{aligned} & \int_{\Omega_j \cap \mathcal{B}_j} b_r(\mathbf{x}_i^\perp)^2 (|\nabla_i f|^2 + \frac{1}{2} v_a(|\mathbf{x}_i - \mathbf{x}_j|) |f|^2) d\mathbf{x}_i \\ & \geq \frac{\min_{\mathbf{x} \in \mathcal{B}_j} b_r(\mathbf{x}^\perp)^2}{\max_{\mathbf{x} \in \mathcal{B}_j} b_r(\mathbf{x}^\perp)^2} a \int_{\Omega_j \cap \mathcal{B}_j} b_r(\mathbf{x}_i^\perp)^2 U(|\mathbf{x}_i - \mathbf{x}_j|) |f|^2. \end{aligned} \quad (8.38)$$

Here  $U$  is given in (2.30). For some  $\delta > 0$  let  $\mathcal{B}_\delta$  be the subset of  $\mathbb{R}^2$  where  $b(\mathbf{x}^\perp)^2 \geq \delta$ , and let  $\chi_{\mathcal{B}_\delta}$  denote its characteristic function. Estimating  $\max_{\mathbf{x} \in \mathcal{B}_j} b_r(\mathbf{x}^\perp)^2 \leq \min_{\mathbf{x} \in \mathcal{B}_j} b_r(\mathbf{x}^\perp)^2 + 2(R/r^3) \|\nabla b^2\|_\infty$ , we obtain

$$\frac{\min_{\mathbf{x} \in \mathcal{B}_j} b_r(\mathbf{x}^\perp)^2}{\max_{\mathbf{x} \in \mathcal{B}_j} b_r(\mathbf{x}^\perp)^2} \geq \chi_{\mathcal{B}_\delta}(\mathbf{x}_j^\perp/r) \left( 1 - 2 \frac{R}{r} \frac{\|\nabla b^2\|_\infty}{\delta} \right). \quad (8.39)$$

Denoting  $k(i)$  the nearest neighbor to particle  $i$ , we conclude that, for  $0 \leq \varepsilon \leq 1$ ,

$$\begin{aligned} & \sum_{i=1}^n \int \left[ |\nabla_i f|^2 + \frac{1}{2} \sum_{j, j \neq i} v_a(|\mathbf{x}_i - \mathbf{x}_j|) |f|^2 \right] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k \\ & \geq \sum_{i=1}^n \int \left[ \varepsilon |\nabla_i f|^2 + (1 - \varepsilon) |\nabla_i f|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i) \right. \\ & \quad \left. + a' U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|) \chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp/r) |f|^2 \right] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k, \end{aligned} \quad (8.40)$$

where  $a' = a(1 - \varepsilon)(1 - 2R\|\nabla b^2\|_\infty/r\delta)$ .

Define  $F(z_1, \dots, z_n) \geq 0$  by

$$|F(z_1, \dots, z_n)|^2 = \int |f(\mathbf{x}_1, \dots, \mathbf{x}_n)|^2 \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k^\perp. \quad (8.41)$$

Neglecting the kinetic energy in  $\perp$ -direction in the second term in (8.40) and using the Schwarz inequality to bound the longitudinal kinetic energy of  $f$  by the one of  $F$ , we get the estimate



$$\begin{aligned}
 \langle \Psi | H | \Psi \rangle &= \frac{ne^\perp}{r^2} \\
 &\geq \sum_{i=1}^n \int \left[ \varepsilon |\partial_i F|^2 + (1 - \varepsilon) |\partial_i F|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i) \right] \prod_{k=1}^n dz_k \\
 &\quad + \sum_{i=1}^n \int \left[ \varepsilon |\nabla_i^\perp f|^2 + a' U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|) \chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp / r) |f|^2 \right] \\
 &\quad \times \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k,
 \end{aligned} \tag{8.42}$$

where  $\partial_j = d/dz_j$ , and  $\nabla^\perp$  denotes the gradient in  $\perp$ -direction. We now investigate the last term in (8.42). Consider, for fixed  $z_1, \dots, z_n$ , the expression

$$\sum_{i=1}^n \int \left[ \varepsilon |\nabla_i^\perp f|^2 + a' U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|) \chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp / r) |f|^2 \right] \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k^\perp. \tag{8.43}$$

To estimate this term from below, we use Temple's inequality, as in Sect. 2.2. Let  $\tilde{\varepsilon}^\perp$  denote the gap above zero in the spectrum of  $-\Delta^\perp + V^\perp - e^\perp$ , i.e., the lowest non-zero eigenvalue. By scaling,  $\tilde{\varepsilon}^\perp / r^2$  is the gap in the spectrum of  $-\Delta^\perp + V_r^\perp - e^\perp / r^2$ . Note that under the transformation  $\phi \mapsto b_r^{-1} \phi$  this latter operator is unitarily equivalent to  $\nabla^{\perp*} \cdot \nabla^\perp$  as an operator on  $L^2(\mathbb{R}^2, b_r(\mathbf{x}^\perp)^2 d\mathbf{x}^\perp)$ , as considered in (8.43). Hence also this operator has  $\tilde{\varepsilon}^\perp / r^2$  as its energy gap. Denoting

$$\langle U^k \rangle = \int \left( \sum_{i=1}^n U(|\mathbf{x}_i - \mathbf{x}_{k(i)}|) \chi_{\mathcal{B}_\delta}(\mathbf{x}_{k(i)}^\perp / r) \right)^k \prod_{k=1}^n b_r(\mathbf{x}_k^\perp)^2 d\mathbf{x}_k^\perp, \tag{8.44}$$

Temple's inequality implies

$$(8.43) \geq |F|^2 a' \langle U \rangle \left( 1 - a' \frac{\langle U^2 \rangle}{\langle U \rangle} \frac{1}{\varepsilon \tilde{\varepsilon}^\perp / r^2 - a' \langle U \rangle} \right). \tag{8.45}$$

Now, using (2.30) and Schwarz's inequality,  $\langle U^2 \rangle \leq 3n(R^3 - R_0^3)^{-1} \langle U \rangle$ , and

$$\langle U \rangle \leq n(n-1) \frac{\|b\|_4^4}{r^2} \frac{3\pi R^2}{R^3 - R_0^3}. \tag{8.46}$$

Therefore

$$(8.45) \geq |F|^2 a'' \langle U \rangle, \tag{8.47}$$

where we put all the error terms into the modified coupling constant  $a''$ . It remains to derive a lower bound on  $\langle U \rangle$ . Let

$$d(z - z') = \int_{\mathbb{R}^4} b_r(\mathbf{x}^\perp)^2 b_r(\mathbf{y}^\perp)^2 U(|\mathbf{x} - \mathbf{y}|) \chi_{\mathcal{B}_\delta}(\mathbf{y}^\perp / r) d\mathbf{x}^\perp d\mathbf{y}^\perp. \tag{8.48}$$

Note that  $d(z) = 0$  if  $|z| \geq R$ . An estimate similar to (2.36) gives

$$\langle U \rangle \geq \sum_{i \neq j} d(z_i - z_j) \left( 1 - (n-2) \frac{\pi R^2}{r^2} \|b\|_\infty^2 \right). \quad (8.49)$$

Note that, for an appropriate choice of  $R$ ,  $d$  is close to a  $\delta$ -function with the desired coefficient. To make the connection with the  $\delta$ -function, we can use a bit of the kinetic energy saved in (8.42) to obtain

$$\begin{aligned} & \int \left[ \frac{\varepsilon}{n-1} |\partial_i F|^2 + a''' d(z_i - z_j) |F|^2 \right] dz_i \\ & \geq \frac{1}{2} g' \max_{|z_i - z_j| \leq R} |F|^2 \chi_{[R, \ell-R]}(z_j) \left( 1 - \left( \frac{2(n-1)}{\varepsilon} g' R \right)^{1/2} \right). \end{aligned} \quad (8.50)$$

Putting all the previous estimates together, we arrive at

$$\begin{aligned} \langle \Psi | H | \Psi \rangle - \frac{ne^\perp}{r^2} & \geq \sum_{i=1}^n \int \left[ (1-\varepsilon) |\partial_i F|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i) \right] \prod_{k=1}^n dz_k \\ & + \sum_{i \neq j} \frac{1}{2} g'' \int \max_{|z_i - z_j| \leq R} |F|^2 \chi_{[R, \ell-R]}(z_j) \prod_{k, k \neq i} dz_k \end{aligned} \quad (8.51)$$

for an appropriate coupling constant  $g''$  that contains all the error terms. Now assume that  $(n+1)R < \ell$ . Given an  $F$  with  $\int |F|^2 dz_1 \cdots dz_n = 1$ , define, for  $0 \leq z_1 \leq z_2 \leq \cdots \leq z_n \leq \ell - (n+1)R$ ,

$$\psi(z_1, \dots, z_n) = F(z_1 + R, z_2 + 2R, z_3 + 3R, \dots, z_n + nR), \quad (8.52)$$

and extend the function to all of  $[0, \ell - (n+1)R]^n$  by symmetry. A simple calculation shows that

$$\begin{aligned} (8.51) & \geq \langle \psi | H' | \psi \rangle \geq (1-\varepsilon) E_N^{\text{1D}}(n, \ell - (n+1)R, g'') \langle \psi | \psi \rangle \\ & \geq (1-\varepsilon) E_N^{\text{1D}}(n, \ell, g'') \langle \psi | \psi \rangle, \end{aligned} \quad (8.53)$$

where  $H'$  is the Hamiltonian (8.3) with a factor  $(1-\varepsilon)$  in front of the kinetic energy term.

It remains to estimate  $\langle \psi | \psi \rangle$ . Using that  $F$  is related to the true ground state  $\Psi$  by (8.41), we can estimate it in terms of the total QM energy, namely

$$\begin{aligned} \langle \psi | \psi \rangle & \geq 1 - \frac{2R}{g''} \left( E_N^{\text{QM}}(N, \ell, r, a) - \frac{ne^\perp}{r^2} \right) \\ & - 2n \frac{R}{\ell} - 4nR \left( \frac{1}{n} E_N^{\text{QM}}(n, \ell, r, a) - \frac{e^\perp}{r^2} \right)^{1/2}. \end{aligned} \quad (8.54)$$

Collecting all the error terms and choosing

$$R = r \left( \frac{a}{r} \right)^{1/4}, \quad \varepsilon = \left( \frac{a}{r} \right)^{1/8}, \quad \delta = \left( \frac{a}{r} \right)^{1/8}, \quad (8.55)$$

(8.53) and (8.54) lead to the desired lower bound.  $\square$

As already noted above, Lemma 8.3 is the key to the proof of Theorems 8.1 and 8.2. The estimates are used in each box, and the particles are distributed optimally among the boxes. For the global lower bound, superadditivity of the energy and convexity of the energy density  $\rho^3 e(g/\rho)$  are used, generalizing corresponding arguments in Sect. 2. We refer to [58] for details.

## 9 The Charged Bose Gas, the One- and Two-Component Cases

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

$$v(|\mathbf{x}_i - \mathbf{x}_j|) = |\mathbf{x}_i - \mathbf{x}_j|^{-1} \tag{9.1}$$

(in 3 dimensions). The unit of electric charge is 1 in our units.

We will here consider both the one- and two-component gases. In the one-component gas (also referred to as the one-component plasma or bosonic jellium) we consider positively charged particles confined to a box with a uniformly charged background. In the two-component gas we have particles of both positive and negative charges moving in all of space.

### 9.1 The One-Component Gas

In the one-component gas there are  $N$  positively charged particles in a large box  $\Lambda$  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  $\rho$ . Our Hamiltonian is thus

$$H_N^{(1)} = \sum_{i=1}^N -\mu \Delta_i - V(\mathbf{x}_i) + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|) + C \tag{9.2}$$

with

$$V(\mathbf{x}) = \rho \int_{\Lambda} |\mathbf{x} - \mathbf{y}|^{-1} d\mathbf{y} \quad \text{and} \quad C = \frac{1}{2} \rho \int_{\Lambda} V(\mathbf{x}) d\mathbf{x} . \tag{9.3}$$

We shall use Dirichlet boundary conditions. As before the Hamiltonian acts on symmetric wave functions in  $L^2(\Lambda^N, d\mathbf{x}_1 \cdots d\mathbf{x}_N)$ .

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  $\Psi = \text{const.}$ ). This time, *large*  $\rho$  is the ‘weakly interacting’ regime.

We know from the work in [50] that the thermodynamic limit  $e_0(\rho)$  defined as in (2.2) exists. It also follows from this work that we would, in fact, get the

same thermodynamic energy if we did not restrict the number of particles  $N$ , but considered the grand-canonical case where we minimize the energy over all possible particle numbers, but keeping the background charge  $\rho$  fixed.

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  $\Psi = \text{const}$ , 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 [23] 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 [60] and [82].

The Bogolubov theory states that the main contribution to the energy comes from pairing of particles into momenta  $\mathbf{k}, -\mathbf{k}$  and is the bosonic analogue of the BCS theory of superconductivity which came a decade later. I.e.,  $\Psi_0$  is a sum of products of terms of the form  $\exp\{i\mathbf{k} \cdot (\mathbf{x}_i - \mathbf{x}_j)\}$ .

The following theorem is the main result for the one-component gas.

**Theorem 9.1 (Foldy's law for the one-component gas).**

$$\lim_{\rho \rightarrow \infty} \rho^{-1/4} e_0(\rho) = -\frac{2}{5} \frac{\Gamma(3/4)}{\Gamma(5/4)} \left( \frac{2}{\mu\pi} \right)^{1/4}. \quad (9.4)$$

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 [48], for which there is no Bose–Einstein condensation.

To appreciate the  $-\rho^{1/4}$  nature of (9.4), it is useful to compare it with what one would get if the bosons had infinite mass, i.e., the first term in (9.2) is dropped. Then the energy would be proportional to  $-\rho^{1/3}$  as shown in [50]. Thus, the effect of quantum mechanics is to lower  $\frac{1}{3}$  to  $\frac{1}{4}$ .

A problem somewhat related to bosonic jellium is *fermionic* jellium. Graf and Solovej [28] have proved that the first two terms are what one would expect, namely

$$e_0(\rho) = C_{\text{TF}}\rho^{5/3} - C_{\text{D}}\rho^{4/3} + o(\rho^{4/3}), \quad (9.5)$$

where  $C_{\text{TF}}$  is the usual Thomas–Fermi constant and  $C_{\text{D}}$  is the usual Dirac exchange constant.

It is supposedly true, for both bosonic and fermionic particles, 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  $\rho$ , and is thus outside the region where a Bogolubov approximation can be expected to hold.

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

Note that in the high density limit  $\ell_{\text{cor}}$  is long compared to the interparticle distance. This is analogous to the dilute gas where the scale  $\ell_c$  is also long compared to the interparticle distance [see (2.12)]. There is however no real analogy between the scale  $\ell_{\text{cor}}$  for the charged gas and the scale  $\ell_c$  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  $e_0(\rho) \not\sim \ell_{\text{cor}}^{-2} = \rho^{1/2}$ . The reason for this difference is that on average only a small fraction of the particles in the charged gas actually correlate.

### 9.2 The Two-Component Gas

Now we consider  $N$  particles with charges  $\pm 1$ . The Hamiltonian is thus

$$H_N^{(2)} = \sum_{i=1}^N -\mu \Delta_i + \sum_{1 \leq i < j \leq N} \frac{e_i e_j}{|\mathbf{x}_i - \mathbf{x}_j|}. \tag{9.6}$$

This time we are interested in  $E_0^{(2)}(N)$  the ground state energy of  $H_N^{(2)}$  minimized over all possible combination of charges  $e_i = \pm 1$ , i.e., we do not necessarily assume that the minimum occurs for the neutral case. Restricting to the neutral case would however not change the result we give below.

An equivalent formulation is to say that  $E_0^{(2)}(N)$  is the ground state energy of the Hamiltonian acting on all wave functions of space and charge, i.e., functions in  $L^2((\mathbb{R}^3 \times \{-1, 1\})^N)$ . As mentioned in the introduction, and explained in the beginning of the proof of Thm. 2.2, for the calculation of the ground state energy we may as usual restrict to symmetric functions in this Hilbert space.

For the two-component gas there is no thermodynamic limit. In fact, Dyson [18] proved that  $E_0^{(2)}(N)$  was at least as negative as  $-(\text{const})N^{7/5}$  as  $N \rightarrow \infty$ .

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 [12], 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 [12]) was pointed out by Dyson [18] 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  $L$  gives  $L \sim N^{-1/5}$  and leads to the  $-N^{7/5}$  law. The correlation length scale is now  $\ell_{\text{cor}} \sim \rho^{-1/4} \sim N^{-2/5}$ .

In [18] Dyson conjectured an exact asymptotic expression for  $E_0^{(2)}(N)$  for large  $N$ . That this asymptotics, as formulated in the next theorem, is indeed correct is proved in [61] and [82].

**Theorem 9.2 (Dyson’s law for the two-component gas).**

$$\lim_{N \rightarrow \infty} \frac{E_0^{(2)}(N)}{N^{7/5}} = \inf \left\{ \mu \int_{\mathbb{R}^3} |\nabla \Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2} \mid 0 \leq \Phi, \int_{\mathbb{R}^3} \Phi^2 = 1 \right\}, \tag{9.7}$$

where  $I_0$  is the constant from Foldy’s law:

$$I_0 = \frac{2}{5} \frac{\Gamma(3/4)}{\Gamma(5/4)} \left( \frac{2}{\mu\pi} \right)^{1/4}. \tag{9.8}$$

This asymptotics can be understood as a mean field theory for the gas density, very much like the Gross–Pitaevskii functional for dilute trapped gases, where the local energy described by Foldy’s law should be balanced by the kinetic energy of the gas density. Thus if we let the gas density be given by  $\phi^2$  then the “mean field” energy should be

$$\mu \int_{\mathbb{R}^3} |\nabla \phi|^2 - I_0 \int_{\mathbb{R}^3} \phi^{5/2}. \tag{9.9}$$

Here  $\int \phi^2 = N$ . If we now define  $\Phi(\mathbf{x}) = N^{-8/5} \phi(N^{-1/5} \mathbf{x})$  we see that  $\int \Phi^2 = 1$  and that the above energy is

$$N^{7/5} \left( \mu \int_{\mathbb{R}^3} |\nabla \Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2} \right). \tag{9.10}$$

It may be somewhat surprising that it is exactly the same constant  $I_0$  that appears in both the one- and two-component cases. The reason that there are no extra factors to account for the difference between one and two components is, as we shall see below, a simple consequence of Bogolubov’s method. The origin of this equivalence, while clear mathematically, does not appear to have a simple physical interpretation.

### 9.3 The Bogolubov Approximation

In this section we shall briefly explain the Bogolubov approximation and how it is applied in the case of the charged Bose gas. The Bogolubov method relies on the exact diagonalization of a Hamiltonian, which is quadratic in creation and annihilation operators. For the charged Bose gas one only needs a very simple case of the general diagonalization procedure. On the other hand, the operators that appear are not exact creation and annihilation operators. A slightly more general formulation is needed.

**Theorem 9.3 (Simple case of Bogolubov’s method).** *Assume that  $b_{\pm,\pm}$  are four (possibly unbounded) commuting operators satisfying the operator inequality*

$$[b_{\tau,e}, b_{\tau,e}^*] \leq 1 \quad \text{for all } e, \tau = \pm. \quad (9.11)$$

Then for all real numbers  $\mathcal{A}, \mathcal{B}_+, \mathcal{B}_- \geq 0$  we have

$$\begin{aligned} & \mathcal{A} \sum_{\tau,e=\pm 1} b_{\tau,e}^* b_{\tau,e} \\ & + \sum_{e,e'=\pm 1} \sqrt{\mathcal{B}_e \mathcal{B}_{e'}} e e' (b_{+,e}^* b_{+,e'} + b_{-,e}^* b_{-,e'} + b_{+,e}^* b_{-,e'}^* + b_{+,e} b_{-,e'}^*) \\ & \geq -(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-) + \sqrt{(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-)^2 - (\mathcal{B}_+ + \mathcal{B}_-)^2}. \end{aligned} \quad (9.12)$$

If  $b_{\pm,\pm}$  are four annihilation operators then the lower bound is sharp.

*Proof.* Let us introduce

$$d_{\pm}^* = (\mathcal{B}_+ + \mathcal{B}_-)^{-1/2} (\mathcal{B}_+^{1/2} b_{\pm,+}^* - \mathcal{B}_-^{1/2} b_{\pm,-}^*), \quad (9.13)$$

and

$$c_{\pm}^* = (\mathcal{B}_+ + \mathcal{B}_-)^{-1/2} (\mathcal{B}_-^{1/2} b_{\pm,+}^* + \mathcal{B}_+^{1/2} b_{\pm,-}^*). \quad (9.14)$$

Then these operators satisfy

$$[d_+, d_+^*] \leq 1, \quad [d_-, d_-^*] \leq 1. \quad (9.15)$$

The operator that we want to estimate from below may be rewritten as

$$\begin{aligned} & \mathcal{A}(d_+^* d_+ + d_-^* d_- + c_+^* c_+ + c_-^* c_-) \\ & + (\mathcal{B}_+ + \mathcal{B}_-) (d_+^* d_+ + d_-^* d_- + d_+^* d_-^* + d_+ d_-). \end{aligned} \quad (9.16)$$

We may now complete the squares to write this as

$$\begin{aligned} & \mathcal{A}(c_+^* c_+ + c_-^* c_-) + D(d_+^* + \lambda d_-)(d_+^* + \lambda d_-)^* \\ & + D(d_-^* + \lambda d_+)(d_-^* + \lambda d_+)^* - D\lambda^2([d_+, d_+^*] + [d_-, d_-^*]) \end{aligned} \quad (9.17)$$

if

$$D(1 + \lambda^2) = \mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-, \quad 2D\lambda = \mathcal{B}_+ + \mathcal{B}_-. \quad (9.18)$$

We choose the solution

$$\lambda = 1 + \frac{\mathcal{A}}{\mathcal{B}_+ + \mathcal{B}_-} - \sqrt{\left(1 + \frac{\mathcal{A}}{\mathcal{B}_+ + \mathcal{B}_-}\right)^2 - 1}. \quad (9.19)$$

Hence

$$D\lambda^2 = \frac{1}{2} \left( \mathcal{A} + \mathcal{B}_+ + \mathcal{B}_- - \sqrt{(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-)^2 - (\mathcal{B}_+ + \mathcal{B}_-)^2} \right). \quad (9.20)$$

□

In the theorem above one could of course also have included linear terms in  $b_{\tau,e}$  in the Hamiltonian. In the technical proofs in [60, 61] the Bogolubov diagonalization with linear terms is indeed being used to control certain error terms. Here we shall not discuss the technical details of the proofs. We have therefore stated the theorem in the simplest form in which we shall need it to derive the leading contribution.

In our applications to the charged Bose gas the operators  $b_{\pm,e}$  will correspond to the annihilation of particles with charge  $e = \pm$  and momenta  $\pm\mathbf{k}$  for some  $\mathbf{k} \in \mathbb{R}^3$ . Thus, only equal and opposite momenta couple. In a translation invariant case this would be a simple consequence of momentum conservation. The one-component gas is not translation invariant, in our formulation. The two-component gas is translation invariant, but it is natural to break translation invariance by going into the center of mass frame. In both cases it is only in some approximate sense that equal and opposite momenta couple.

In the case of the one-component gas we only need particles of one sign. In this case we use the above theorem with  $b_{\pm,-} = 0$  and  $\mathcal{B}_- = 0$ .

We note that the lower bounds in Theorem 9.3 for the one- and two-component gases are the same except for the replacement of  $\mathcal{B}_+$  in the one-component case by  $\mathcal{B}_+ + \mathcal{B}_-$  in the two-component case. In the application to the two-component gas  $\mathcal{B}_+$  and  $\mathcal{B}_-$  will be proportional to the particle densities for respectively the positive or negatively charged particles. For the one-component gas  $\mathcal{B}_+$  is proportional to the background density.

The Bogolubov diagonalization method cannot be immediately applied to the operators  $H_N^{(1)}$  or  $H_N^{(2)}$  since these operators are *not* quadratic in creation and annihilation operators. In fact, they are quartic. They have the general form

$$\sum_{\alpha,\beta} t_{\alpha\beta} a_\alpha^* a_\beta + \frac{1}{2} \sum_{\alpha,\beta,\mu,\nu} w_{\alpha\beta\mu\nu} a_\alpha^* a_\beta^* a_\nu a_\mu, \quad (9.21)$$

with

$$t_{\alpha\beta} = \langle \alpha | T | \beta \rangle, \quad w_{\alpha\beta\mu\nu} = \langle \alpha\beta | W | \mu\nu \rangle, \quad (9.22)$$

where  $T$  is the one-body part of the Hamiltonian and  $W$  is the two-body-part of the Hamiltonian.



The main step in Bogolubov's approximation is now to assume Bose-Einstein condensation, i.e., that almost all particles are in the same one-particle state. In case of the two-component gas this means that almost half the particles are positively charged and in the same one-particle state as almost all the other half of negatively charged particles. We denote this condensate state by the index  $\alpha = 0$  in the sums above. Based on the assumption of condensation Bogolubov now argues that one may ignore all terms in the quartic Hamiltonian above which contain 3 or 4 non-zero indices and at the same time replace all creation and annihilation operators of the condensate by their expectation values. The result is a quadratic Hamiltonian (including linear terms) in the creation and annihilation with non-zero index. This Hamiltonian is of course not particle number preserving, reflecting the simple fact that particles may be created out of the condensate or annihilated into the condensate.

In Sect. 9.5 below it is explained how to construct trial wave functions for the one- and two-component charged gases whose expectations agree essentially with the prescription in the Bogolubov approximation. The details are to appear in [82]. This will imply upper bounds on the energies corresponding to the asymptotic forms given in Theorems 9.1 and 9.2.

In [60, 61] it is proved how to make the steps in the Bogolubov approximation rigorous as lower bounds. The main difficulty is to control the degree of condensation. As already explained it is not necessary to prove condensation in the strong sense described above. We shall only prove condensation in small boxes. Put differently, we shall not conclude that most particles are in the same one-particle state, but rather prove that most particles occupy one-particle states that look the same on short scales, i.e., that vary slowly. Here the short scale is the correlation length scale  $\ell_{\text{cor}}$ .

#### 9.4 The Rigorous Lower Bounds

As already mentioned we must localize into small boxes of some fixed size  $\ell$ . This time we must require  $\ell_{\text{cor}} \ll \ell$ . For the one-component gas this choice is made only in order to control the degree of condensation. For the two-component gas it is required both to control the order of condensation, and also to make a local constant density approximation. The reason we can control the degree of condensation in a small box is that the localized kinetic energy has a gap above the lowest energy state. In fact, the gap is of order  $\ell^{-2}$ . Thus if we require that  $\ell$  is such that  $N\ell^{-2}$  is much greater than the energy we may conclude that most particles are in the lowest eigenvalue state for the localized kinetic energy. We shall always choose the localized kinetic energy in such a way that the lowest eigenstate, and hence the condensate, is simply a constant function.

## Localizing the Interaction

In contrast to the dilute gas the long range Coulomb potential prevents us from simply ignoring the interaction between the small boxes. To overcome this problem we use a sliding technique first introduced in [12].

**Theorem 9.4 (Controlling interactions by sliding).** *Let  $\chi$  be a smooth approximation to the characteristic function of the unit cube centered at the origin. For  $\ell > 0$  and  $\mathbf{z} \in \mathbb{R}^3$  let  $\chi_{\mathbf{z}}(\mathbf{x}) = \chi((\mathbf{x} - \mathbf{z})/\ell)$ . There exists an  $\omega > 0$  depending on  $\chi$  (in such a way that it tends to infinity as  $\chi$  approximates the characteristic function) such that*

$$\sum_{1 \leq i < j \leq N} \frac{e_i e_j}{|\mathbf{x}_i - \mathbf{x}_j|} \geq \left( \int \chi^2 \right)^{-1} \int_{\mathbb{R}^3} \sum_{1 \leq i < j \leq N} e_i e_j w_{\ell \mathbf{z}}(\mathbf{x}_i, \mathbf{x}_j) d\mathbf{z} - \frac{N\omega}{2\ell}, \quad (9.23)$$

for all  $\mathbf{x}_1, \dots \in \mathbb{R}^3$  and  $e_1, \dots = \pm 1$ , where

$$w_{\mathbf{z}}(\mathbf{x}, \mathbf{y}) = \chi_{\mathbf{z}}(\mathbf{x}) Y_{\omega/\ell}(\mathbf{x} - \mathbf{y}) \chi_{\mathbf{z}}(\mathbf{y}) \quad (9.24)$$

with  $Y_{\mu}(\mathbf{x}) = |\mathbf{x}|^{-1} \exp(-\mu|\mathbf{x}|)$  being the Yukawa potential.

The significance of this result is that the two-body potential  $w_{\mathbf{z}}$  is localized to the cube of size  $\ell$  centered at  $\ell \mathbf{z}$ . The lower bound above is thus an integral over localized interactions sliding around with the integration parameter.

We have stated the sliding estimate in the form relevant to the two-component problem. There is an equivalent version for the one-component gas, where the sum of the particle-particle, particle-background, and background-background interactions may be bounded below by corresponding localized interactions.

Since  $\ell \gg \ell_{\text{cor}}$  the error in the sliding estimate is much smaller than  $\omega N/\ell_{\text{cor}}$ , which for both the one and two-component gases is of order  $\omega$  times the order of the energy. Thus, since  $\ell$  is much bigger than  $\ell_{\text{cor}}$ , we have room to let  $\omega$  be very large, i.e.,  $\chi$  is close to the characteristic function.

## Localizing the Kinetic Energy

Having described the technique to control the interaction between localized regions we turn next to the *localization of the kinetic energy*.

For the two-component gas this is done in two steps. As already mentioned it is natural to break the translation invariance of the two-component gas. We do this by localizing the system into a box of size  $L' \gg N^{-1/5}$  (which as we saw is the expected size of the gas) as follows. By a partition of unity we can divide space into boxes of this size paying a localization error due to the kinetic energy of order  $NL'^{-2} \ll N^{7/5}$ . We control the interaction between these boxes using the sliding technique.

We may now argue, as follows, that the energy is smallest if all the particles are in just one box. For simplicity we give this argument for the case of two boxes. Suppose the two boxes have respective wave functions  $\psi$  and  $\tilde{\psi}$ . The total energy of these two non-interacting boxes is  $E + \tilde{E}$ . Now put all the particles in one box with the trial function  $\Psi = \psi\tilde{\psi}$ . The fact that this function is not bosonic (i.e., it is not symmetric with respect to all the variables) is irrelevant because the true bosonic ground state energy is never greater than that of any trial state (Perron–Frobenius Theorem). The energy of  $\Psi$  is

$$E + \tilde{E} + \iint \rho_\psi(\mathbf{x})|\mathbf{x} - \mathbf{y}|^{-1}\rho_{\tilde{\psi}}(\mathbf{y})d\mathbf{x}d\mathbf{y} , \tag{9.25}$$

where  $\rho_\psi$  and  $\rho_{\tilde{\psi}}$  are the respective *charge densities* of the states  $\psi$  and  $\tilde{\psi}$ . We claim that the last Coulomb term can be made non-positive. How? If it is positive then we simply change the state  $\tilde{\psi}$  by interchanging positive and negative charges (only in  $\tilde{\psi}$  and not in  $\psi$ ). The reader is reminded that we have not constrained the number of positive and negative particles but only their sum. This change in  $\tilde{\psi}$  reverses the relative charge of the states  $\psi$  and  $\tilde{\psi}$  so, by symmetry the energies  $E$  and  $\tilde{E}$  do not change, whereas the Coulomb interaction changes sign.

The localization into smaller cubes of size  $\ell$  can however not be done by a crude partition of unity localization. Indeed, this would cost a localization error of order  $N\ell^{-2}$ , which as explained is required to be of much greater order than the energy.

For the one-component charged gas we may instead use a Neumann localization of the kinetic energy, as for the dilute Bose gas. If we denote by  $\Delta_\ell^{(\mathbf{z})}$  the Neumann Laplacian for the cube of size  $\ell$  centered at  $\mathbf{z}$  we may, in the spirit of the sliding estimate, write the Neumann localization Laplacian in all of  $\mathbb{R}^3$  as

$$-\Delta = \int -\Delta_\ell^{(\ell\mathbf{z})}d\mathbf{z} . \tag{9.26}$$

In order to write the localized kinetic energy in the same form as the localized interaction we must introduce the smooth localization  $\chi$  as in Theorem 9.4. This can be achieved by ignoring the low momentum part of the kinetic energy.

More precisely, there exist  $\varepsilon(\chi)$  and  $s(\chi)$  such that  $\varepsilon(\chi) \rightarrow 0$  and  $s(\chi) \rightarrow 0$  as  $\chi$  approaches the characteristic function of the unit cube and such that (see Lemma 6.1 in [60])

$$-\Delta_\ell^{(\mathbf{z})} \geq (1 - \varepsilon(\chi))\mathcal{P}_\mathbf{z}\chi_\mathbf{z}(\mathbf{x})F_{\ell s(\chi)}(-\Delta)\chi_\mathbf{z}(\mathbf{x})\mathcal{P}_\mathbf{z} \tag{9.27}$$

where  $\mathcal{P}_\mathbf{z}$  denotes the projection orthogonal to constants in the cube of size  $\ell$  centered at  $\mathbf{z}$  and

$$F_s(u) = \frac{u^2}{u + s^{-2}} . \tag{9.28}$$

For  $u \ll s^{-2}$  we have that  $F_s(u) \ll u$ . Hence the effect of  $F$  in the operator estimate above is to ignore the low momentum part of the Laplacian.

For the two-component gas one cannot use the Neumann localization as for the one-component gas. Using a Neumann localization ignores the kinetic energy corresponding to long range variations in the wave function and one would not get the kinetic energy term  $\int \mu |\nabla \Phi|^2$  in (9.7). This is the essential difference between the one- and two-component cases. This problem is solved in [61] where a new kinetic energy localization technique is developed. The idea is again to separate the high and low momentum part of the kinetic energy. The high momentum part is then localized as before, whereas the low momentum part is used to connect the localized regions by a term corresponding to a discrete Laplacian. (For details and the proof the reader is referred to [61].)

**Theorem 9.5 (A many body kinetic energy localization).** *Let  $\chi_{\mathbf{z}}$ ,  $\mathcal{P}_{\mathbf{z}}$  and  $F_s$  be as above. There exist  $\varepsilon(\chi)$  and  $s(\chi)$  such that  $\varepsilon(\chi) \rightarrow 0$  and  $s(\chi) \rightarrow 0$  as  $\chi$  approaches the characteristic function of the unit cube and such that for all normalized symmetric wave functions  $\Psi$  in  $L^2((\mathbb{R}^3 \times \{-1, 1\})^N)$  and all  $\Omega \subset \mathbb{R}^3$  we have*

$$\begin{aligned}
 (1 + \varepsilon(\chi)) \left( \Psi, \sum_{i=1}^N -\Delta_i \Psi \right) &\geq \int_{\Omega} \left[ (\Psi, \mathcal{P}_{\ell \mathbf{z}} \chi_{\ell \mathbf{z}}(\mathbf{x}) F_{\ell s(\chi)}(-\Delta) \chi_{\ell \mathbf{z}}(\mathbf{x}) \mathcal{P}_{\ell \mathbf{z}} \Psi) \right. \\
 &\quad \left. + \frac{1}{2} \ell^{-2} \sum_{\substack{\mathbf{y} \in \mathbb{Z}^3 \\ |\mathbf{y}|=1}} (S_{\Psi}(\ell(\mathbf{z} + \mathbf{y})) - S_{\Psi}(\ell \mathbf{z}))^2 \right] d\mathbf{z} \\
 &\quad - \text{const. } \ell^{-2} \text{Vol}(\Omega) ,
 \end{aligned} \tag{9.29}$$

where

$$S_{\Psi}(\mathbf{z}) = \sqrt{(\Psi, (a_{0+}^*(\mathbf{z})a_{0+}(\mathbf{z}) + a_{0-}^*(\mathbf{z})a_{0-}(\mathbf{z}))\Psi) + 1} - 1 \tag{9.30}$$

with  $a_{0\pm}(z)$  being the annihilation of a particle of charge  $\pm$  in the state given by the normalized characteristic function of the cube of size  $\ell$  centered at  $\mathbf{z}$ .

The first term in the kinetic energy localization in this theorem is the same as in (9.27). The second term gives rise to a discrete Laplacian for the function  $S_{\Psi}(\ell \mathbf{z})$ , which is essentially the number of condensate particles in the cube of size  $\ell$  centered at  $\ell \mathbf{z}$ . Since we will eventually conclude that most particles are in the condensate this term will after approximating the discrete Laplacian by the continuum Laplacian lead to the term  $\int \mu |\nabla \phi|^2$  in (9.9). We shall not discuss this any further here.

When we apply this theorem to the two-component gas the set  $\ell \Omega$  will be the box of size  $L'$  discussed above. Hence the error term  $\ell^{-2} \text{Vol}(\Omega)$  will be of order  $L'^3/\ell^{-5} \ll (N^{2/5} \ell)^{-5} (N^{1/5} L')^3 N^{7/5}$ . Thus since  $\ell \gg N^{-2/5}$  we may still choose  $L' \gg N^{-1/5}$ , as required, and have this error term be lower order than  $N^{7/5}$ .

### Controlling the Degree of Condensation

After now having localized the problem into smaller cubes we are ready to control the degree of condensation. We recall that the condensate state is the constant function in each cube. Let us denote by  $\hat{n}_{\mathbf{z}}$  the number of excited (i.e., non-condensed particles) in the box of size  $\ell$  centered at  $\mathbf{z}$ . Thus for the two-component gas  $\hat{n}_{\mathbf{z}} + a_{0+}^*(\mathbf{z})a_{0+}(\mathbf{z}) + a_{0-}^*(\mathbf{z})a_{0-}(\mathbf{z})$  is the total number of particles in the box and a similar expression gives the particle number for the one-component gas.

As discussed above we can use the fact that the kinetic energy localized to a small box has a gap above its lowest eigenvalue to control the number of excited particles. Actually, this will show that the expectation  $(\Psi, \hat{n}_{\mathbf{z}}\Psi)$  is much smaller than the total number of particles in the box for any state  $\Psi$  with negative energy expectation.

One needs, however, also a good bound on  $(\Psi, \hat{n}_{\mathbf{z}}^2\Psi)$  to control the Coulomb interaction of the non-condensed particles. This is more difficult. In [60] this is not achieved directly through a bound on  $(\Psi, \hat{n}_{\mathbf{z}}\Psi)$  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  $\hat{n}_{\mathbf{z}}$  localized close to  $(\Psi, \hat{n}_{\mathbf{z}}\Psi)$ . The following theorem gives this very general localization technique. Its proof can be found in [60].

**Theorem 9.6 (Localizing large matrices).** *Suppose that  $\mathcal{A}$  is an  $N + 1 \times N + 1$  Hermitean matrix and let  $\mathcal{A}^k$ , with  $k = 0, 1, \dots, N$ , denote the matrix consisting of the  $k^{\text{th}}$  supra- and infra-diagonal of  $\mathcal{A}$ . Let  $\psi \in \mathbf{C}^{N+1}$  be a normalized vector and set  $d_k = (\psi, \mathcal{A}^k\psi)$  and  $\lambda = (\psi, \mathcal{A}\psi) = \sum_{k=0}^N d_k$ . ( $\psi$  need not be an eigenvector of  $\mathcal{A}$ .)*

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

$$(\phi, \mathcal{A}\phi) \leq \lambda + \frac{C}{M^2} \sum_{k=1}^{M-1} k^2 |d_k| + C \sum_{k=M}^N |d_k|, \tag{9.31}$$

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

To use this theorem we start with a ground state (or approximate ground state)  $\Psi$  to the many body problem. We then consider the projections of  $\Psi$  onto the eigenspaces of  $\hat{n}_{\mathbf{z}}$ . Since the possible eigenvalues run from 0 to  $N$  these projections span an at most  $N + 1$  dimensional space.

We use the above theorem with  $\mathcal{A}$  being the many body Hamiltonian restricted to this  $N + 1$  dimensional subspace. Since the Hamiltonian can change the number of excited particles by at most two we see that  $d_k$  vanishes for  $k \geq 3$ . We shall not here discuss the estimates on  $d_1$  and  $d_2$  (see [60, 61]). The conclusion is that we may, without changing the energy expectation of

$\Psi$  too much, assume that the values of  $\widehat{n}_{\mathbf{z}}$  run in an interval of length much smaller than the total number of particles. We would like to conclude that this interval is close to zero. This follows from the fact that any wave function with energy expectation close to the minimum must have an expected number of excited particles much smaller than the total number of particles.

### The Quadratic Hamiltonian

Using our control on the degree of condensation it is now possible to estimate all unwanted terms in the Hamiltonian, i.e., terms that contain 3 or more creation or annihilation operators corresponding to excited (non-condensate) states. The proof which is a rather complicated bootstrapping argument is more or less the same for the one- and two-component gases. The result, in fact, shows that we can ignore other terms too. In fact if we go back to the general form (9.21) of the Hamiltonian it turns out that we can control all quartic terms except the ones with the coefficients:

$$w_{\alpha\beta 00}, w_{00\alpha\beta}, w_{\alpha 00\beta}, \text{ and } w_{0\alpha\beta 0} . \tag{9.32}$$

To be more precise, let  $u_\alpha, \alpha = 1, \dots$  be an orthonormal basis of real functions for the subspace of functions on the cube of size  $\ell$  centered at  $\mathbf{z}$  orthogonal to constants, i.e, with vanishing average in the cube. We shall now omit the subscript  $\mathbf{z}$  and let  $a_{0\pm}$  be the annihilation of a particle of charge  $\pm 1$  in the normalized constant function in the cube (i.e., in the condensate). Let  $a_{\alpha\pm}$  with  $\alpha \neq 0$  be the annihilation operator for a particle of charge  $\pm 1$  in the state  $u_\alpha$ . We can then show that the main contribution to the localized energy of the two-component gas comes from the Hamiltonian

$$\begin{aligned}
 H_{\text{local}} = & \sum_{\substack{\alpha, \beta=1 \\ e=\pm 1}}^{\infty} t_{\alpha\beta} a_{\alpha e}^* a_{\beta e} \\
 & + \frac{1}{2} \sum_{\substack{\alpha, \beta=1 \\ e, e'=\pm 1}} e e' w_{\alpha\beta} (2 a_{0e}^* a_{\alpha e'}^* a_{0e'} a_{\beta e} + a_{0e}^* a_{0e'}^* a_{\alpha e'} a_{\beta e} + a_{\alpha e}^* a_{\beta e'}^* a_{0e'} a_{0e}) ,
 \end{aligned} \tag{9.33}$$

where

$$t_{\alpha\beta} = \mu(u_\alpha, \mathcal{P}_{\mathbf{z}} \chi_{\mathbf{z}}(\mathbf{x}) F_{\ell s(\chi)}(-\Delta) \chi_{\mathbf{z}}(\mathbf{x}) \mathcal{P}_{\mathbf{z}} u_\beta) \tag{9.34}$$

and

$$w_{\alpha\beta} = \ell^{-3} \iint u_\alpha(\mathbf{x}) \chi_{\mathbf{z}}(\mathbf{x}) Y_{\omega/\ell}(\mathbf{x} - \mathbf{y}) \chi_{\mathbf{z}}(\mathbf{y}) u_\beta(\mathbf{x}) d\mathbf{x} d\mathbf{y} . \tag{9.35}$$

In  $H_{\text{local}}$  we have ignored all error terms and hence also  $\varepsilon(\chi) \approx 0$  and  $\int \chi^2 \approx 1$ .

In the case of the one-component gas we get exactly the same local Hamiltonian, except that we have only one type of particles, i.e, we may set  $a_{\alpha-} = 0$  above.

Let  $\nu_{\pm} = \sum_{\alpha=0}^{\infty} a_{\alpha\pm}^* a_{\alpha\pm}$  be the total number of particles in the box with charge  $\pm 1$ . For  $\mathbf{k} \in \mathbb{R}^3$  we let  $\chi_{\mathbf{k},\mathbf{z}}(\mathbf{x}) = \chi_{\mathbf{z}}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$ . We then introduce the operators

$$b_{\mathbf{k}\pm} = (\ell^3 \nu_{\pm})^{-1/2} a_{\pm}(\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{k},\mathbf{z}}) a_{0\pm}^* , \tag{9.36}$$

where  $a_{\pm}(\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{k},\mathbf{z}}) = \sum_{\alpha=1}^{\infty} (\chi_{\mathbf{k},\mathbf{z}}, u_{\alpha}) a_{\alpha\pm}$  annihilates a particle in the state  $\chi_{\mathbf{k},\mathbf{z}}$  with charge  $\pm 1$ . It is then clear that the operators  $b_{\mathbf{k}\pm}$  all commute and a straightforward calculation shows that

$$[b_{\mathbf{k}\pm}, b_{\mathbf{k}\pm}^*] \leq (\ell^3 \nu_{\pm})^{-1} \|\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{z}}\|^2 a_{0\pm}^* a_{0\pm} \leq 1 . \tag{9.37}$$

If we observe that

$$\begin{aligned} \sum_{\substack{\alpha,\beta=1 \\ e=\pm 1}}^{\infty} t_{\alpha\beta} a_{\alpha e}^* a_{\beta e} &= (2\pi)^{-3} \int \mu F_{\ell s(\chi)}(\mathbf{k}^2) \sum_{e=\pm} a_e(\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{k},\mathbf{z}})^* a_e(\mathcal{P}_{\mathbf{z}} \chi_{\mathbf{k},\mathbf{z}}) d\mathbf{k} \\ &\geq (2\pi)^{-3} \ell^3 \int \mu F_{\ell s(\chi)}(\mathbf{k}^2) \sum_{e=\pm} b_{\mathbf{k}e}^* b_{\mathbf{k}e} , \end{aligned} \tag{9.38}$$

we see that

$$\begin{aligned} H_{\text{local}} &\geq \frac{1}{2} (2\pi)^{-3} \int \left[ \mu \ell^3 F_{\ell s(\chi)}(\mathbf{k}^2) \sum_{e=\pm} (b_{\mathbf{k}e}^* b_{\mathbf{k}e} + b_{-\mathbf{k}e}^* b_{-\mathbf{k}e}) \right. \\ &\quad \left. + \sum_{e,e'=\pm} \widehat{Y}_{\omega/\ell}(\mathbf{k}) \sqrt{\nu_e \nu_{e'}} e e' (b_{\mathbf{k}e}^* b_{\mathbf{k},e'} + b_{-\mathbf{k}e}^* b_{-\mathbf{k},e'} + b_{\mathbf{k}e}^* b_{-\mathbf{k},e'}^* + b_{-\mathbf{k}e}^* b_{\mathbf{k},e'}) \right] d\mathbf{k} \\ &\quad - \sum_{\alpha\beta=1} w_{\alpha\beta} (a_{\alpha+}^* a_{\beta+} + a_{\alpha-}^* a_{\beta-}) \end{aligned} \tag{9.39}$$

The last term comes from commuting  $a_{0\pm}^* a_{0\pm}$  to  $a_{0\pm} a_{0\pm}^*$ . It is easy to see that this last term is a bounded operator with norm bounded by

$$\text{const.} (\nu_+ + \nu_-) \ell^{-3} \|\widehat{Y}_{\omega/\ell}\|_{\infty} \leq \text{const.} \omega^{-2} (\nu_+ + \nu_-) \ell^{-1} . \tag{9.40}$$

When summing over all boxes we see that the last term above gives a contribution bounded by  $\text{const.} \omega^{-2} N \ell^{-1} = \omega^{-2} (N^{2/5} \ell)^{-1} N^{7/5}$  which is lower order than the energy.

The integrand in the lower bound on  $H_{\text{local}}$  is precisely an operator of the form treated in the Bogolubov method Theorem 9.3. Thus up to negligible errors we see that the operator  $H_{\text{local}}$  is bounded below by

$$\frac{1}{2} (2\pi)^{-3} \int -(\mathcal{A}(\mathbf{k}) + \mathcal{B}(\mathbf{k})) + \sqrt{(\mathcal{A}(\mathbf{k}) + \mathcal{B}(\mathbf{k}))^2 - \mathcal{B}(\mathbf{k})^2} d\mathbf{k} , \tag{9.41}$$

where

$$\mathcal{A}(\mathbf{k}) = \mu \ell^3 F_{\ell s(\chi)}(\mathbf{k}^2) \quad \text{and} \quad \mathcal{B}(\mathbf{k}) = \nu \widehat{Y}_{\omega/\ell}(\mathbf{k}) \tag{9.42}$$

with  $\nu = \nu_+ + \nu_-$  being the total number of particles in the small box. A fairly simple analysis of the above integral shows that we may to leading

order replace  $\mathcal{A}$  by  $\mu\ell^3\mathbf{k}^2$  and  $\mathcal{B}(\mathbf{k})$  by  $4\pi\nu|\mathbf{k}|^{-2}$ , i.e., we may ignore the cut-offs. The final conclusion is that the local energy is given to leading order by

$$\begin{aligned} & \frac{-1}{2(2\pi)^3} \int 4\pi\nu|\mathbf{k}|^{-2} + \mu\ell^3|\mathbf{k}|^2 - \sqrt{(4\pi\nu|\mathbf{k}|^{-2} + \mu\ell^3|\mathbf{k}|^2)^2 - (4\pi\nu|\mathbf{k}|^{-2})^2} \, d\mathbf{k} \\ & = -2^{1/2}\pi^{-3/4}\nu \left(\frac{\nu}{\mu\ell^3}\right)^{1/4} \int_0^\infty 1 + x^4 - x^2(2 + x^4)^{1/2} \, dx. \quad (9.43) \end{aligned}$$

If we finally use that

$$\int_0^\infty 1 + x^4 - x^2(2 + x^4)^{1/2} \, dx = \frac{2^{3/4}\sqrt{\pi}\Gamma(3/4)}{5\Gamma(5/4)} \quad (9.44)$$

we see that the local energy to leading order is  $-I_0\nu(\nu/\ell^3)^{1/4}$ . For the one-component gas we should set  $\nu = \rho\ell^3$  and for the two-component gas we should set  $\nu = \phi^2\ell^3$  (see (9.9)). After replacing the sum over boxes by an integral and at the same time replace the discrete Laplacian by a continuum Laplacian, as described above, we arrive at asymptotic lower bounds as in Theorems 9.1 and 9.2.

There is one issue that we have not discussed at all and which played an important role in the treatment of the dilute gas. How do we know the number of particles in each of the small cubes? For the dilute gas a superadditivity argument was used to show that there was an equipartition of particles among the smaller boxes. Such an argument cannot be used for the charged gas. For the one-component gas one simply minimizes the energy over all possible particle numbers in each little box. It turns out that charge neutrality is essentially required for the energy to be minimized. Since the background charge in each box is fixed this fixes the particle number.

For the two-component there is a-priori nothing that fixes the particle number in each box. More precisely, if we ignored the kinetic energy between the small boxes it would be energetically favorable to put all particles in one small box. It is the kinetic energy between boxes, i.e., the discrete Laplacian term in Theorem 9.5, that prevents this from happening. Thus we could in principle again minimize over all particle numbers and hope to prove the correct particle number dependence (i.e., Foldy's law) in each small box. This is essentially what is done except that boxes with very many or very few particles must be treated somewhat differently from the "good" boxes. In the "bad" boxes we do not prove Foldy's law, but only weaker estimates that are adequate for the argument.



### 9.5 The Rigorous Upper Bounds

#### The Upper Bound for the Two-component Gas

To prove an upper bound on the energy  $E_0^{(2)}(N)$  of the form given in Dyson's formula Theorem 9.2 we shall construct a trial function from the prescription in the Bogolubov approximation. We shall use as an input a minimizer  $\Phi$  for the variational problem on the right side of (9.7). That minimizers exist can be easily seen using spherical decreasing rearrangements. It is however not important that a minimizer exists. An approximate minimizer would also do for the argument given here. Define  $\phi_0(\mathbf{x}) = N^{3/10}\Phi(N^{1/5}\mathbf{x})$ . Then again  $\int \phi_0^2 = 1$ . In terms of the unscaled function  $\phi$  in (9.9),  $\phi_0(\mathbf{x}) = N^{-1}\phi(\mathbf{x})$ .

Let  $\phi_\alpha, \alpha = 1, \dots$  be an orthonormal family of real functions all orthogonal to  $\phi_0$ . We choose these functions below.

We follow Dyson [18] and choose a trial function which does not have a specified particle number, i.e., a state in the bosonic Fock space.

As our trial many-body wave function we now choose

$$\begin{aligned} \Psi = & \exp\left(-\lambda_0^2 + \lambda_0 a_{0+}^* + \lambda_0 a_{0-}^*\right) \\ & \times \prod_{\alpha \neq 0} (1 - \lambda_\alpha^2)^{1/4} \exp\left(-\sum_{e, e' = \pm 1} \sum_{\alpha \neq 0} \frac{\lambda_\alpha}{4} ee' a_{\alpha, e}^* a_{\alpha, e'}^*\right) |0\rangle, \end{aligned} \tag{9.45}$$

where  $a_{\alpha, e}^*$  is the creation of a particle of charge  $e = \pm 1$  in the state  $\phi_\alpha$ ,  $|0\rangle$  is the vacuum state, and the coefficients  $\lambda_0, \lambda_1, \dots$  will be chosen below satisfying  $0 < \lambda_\alpha < 1$  for  $\alpha \neq 0$ .

It is straightforward to check that  $\Psi$  is a normalized function.

Dyson used a very similar trial state in [18], but in his case the exponent was a purely quadratic expression in creation operators, whereas the one used here is only quadratic in the creation operators  $a_{\alpha e}^*$ , with  $\alpha \neq 0$  and linear in  $a_{0\pm}^*$ . As a consequence our state will be more sharply localized around the mean of the particle number.

In fact, the above trial state is precisely what is suggested by the Bogolubov approximation. To see this note that one has

$$(a_{0\pm} - \lambda_0)\Psi = 0, \quad \text{and} \quad (a_{\alpha+}^* - a_{\alpha-}^* + \lambda_\alpha(a_{\alpha+} - a_{\alpha-}))\Psi = 0 \tag{9.46}$$

for all  $\alpha \neq 0$ . Thus the creation operators for the condensed states can be replaced by their expectation values and an adequate quadratic expression in the non-condensed creation and annihilation operators is minimized.

Consider now the operator

$$\gamma = \sum_{\alpha=1}^{\infty} \frac{\lambda_\alpha^2}{1 - \lambda_\alpha^2} |\phi_\alpha\rangle \langle \phi_\alpha|. \tag{9.47}$$

A straightforward calculation of the energy expectation in the state  $\Psi$  gives that

$$\begin{aligned} \left( \Psi, \sum_{N=0}^{\infty} H_N^{(2)} \Psi \right) &= 2\lambda_0^2 \mu \int (\nabla \phi_0)^2 + \text{Tr}(-\mu \Delta \gamma) \\ &+ 2\lambda_0^2 \text{Tr} \left( \mathcal{K} \left( \gamma - \sqrt{\gamma(\gamma + 1)} \right) \right), \end{aligned} \tag{9.48}$$

where  $\mathcal{K}$  is the operator with integral kernel

$$\mathcal{K}(\mathbf{x}, \mathbf{y}) = \phi_0(\mathbf{x}) |\mathbf{x} - \mathbf{y}|^{-1} \phi_0(\mathbf{y}). \tag{9.49}$$

Moreover, the expected particle number in the state  $\Psi$  is  $2\lambda_0^2 + \text{Tr}(\gamma)$ . In order for  $\Psi$  to be well defined by the formula (9.45) we must require this expectation to be finite.

Instead of making explicit choices for the individual functions  $\phi_\alpha$  and the coefficients  $\lambda_\alpha$ ,  $\alpha \neq 0$  we may equivalently choose the operator  $\gamma$ . In defining  $\gamma$  we use the method of coherent states. Let  $\chi$  be a non-negative real and smooth function supported in the unit ball in  $\mathbb{R}^3$ , with  $\int \chi^2 = 1$ . Let as before  $N^{-2/5} \ll \ell \ll N^{-1/5}$  and define  $\chi_\ell(\mathbf{x}) = \ell^{-3/2} \chi(\mathbf{x}/\ell)$ . We choose

$$\gamma = (2\pi)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(\mathbf{u}, |\mathbf{p}|) \mathcal{P}_{\phi_0}^\perp |\theta_{\mathbf{u}, \mathbf{p}}\rangle \langle \theta_{\mathbf{u}, \mathbf{p}}| \mathcal{P}_{\phi_0}^\perp d\mathbf{u} d\mathbf{p} \tag{9.50}$$

where  $\mathcal{P}_{\phi_0}^\perp$  is the projection orthogonal to  $\phi_0$ ,

$$\theta_{\mathbf{u}, \mathbf{p}}(x) = \exp(i\mathbf{p} \cdot \mathbf{x}) \chi_\ell(\mathbf{x} - \mathbf{u}), \tag{9.51}$$

and

$$f(\mathbf{u}, |\mathbf{p}|) = \frac{1}{2} \left( \frac{\mathbf{p}^4 + 16\pi\lambda_0^2\mu^{-1}\phi_0(\mathbf{u})^2}{\mathbf{p}^2(\mathbf{p}^4 + 32\pi\lambda_0^2\mu^{-1}\phi_0(\mathbf{u})^2)^{1/2}} - 1 \right). \tag{9.52}$$

We note that  $\gamma$  is a positive trace class operator,  $\gamma\phi_0 = 0$ , and that all eigenfunctions of  $\gamma$  may be chosen real. These are precisely the requirements needed in order for  $\gamma$  to define the orthonormal family  $\phi_\alpha$  and the coefficients  $\lambda_\alpha$  for  $\alpha \neq 0$ .

We use the following version of the Berezin–Lieb inequality [5, 46]. Assume that  $\xi(t)$  is an *operator* concave function of  $\mathbb{R}_+ \cup \{0\}$  with  $\xi(0) \geq 0$ . Then if  $Y$  is a positive semi-definite operator we have

$$\text{Tr}(Y\xi(\gamma)) \geq (2\pi)^{-3} \int \xi(f(\mathbf{u}, |\mathbf{p}|)) (\theta_{\mathbf{u}, \mathbf{p}}, \mathcal{P}_{\phi_0}^\perp Y \mathcal{P}_{\phi_0}^\perp \theta_{\mathbf{u}, \mathbf{p}}) d\mathbf{u} d\mathbf{p}. \tag{9.53}$$

We use this for the function  $\xi(t) = \sqrt{t(t+1)}$ . Of course, if  $\xi$  is the identity function then (9.53) is an identity. If  $Y = I$  then (9.53) holds for all concave  $\xi$  with  $\xi(0) \geq 0$ .

Proving an upper bound on the energy expectation (9.48) is thus reduced to the calculations of explicit integrals. After estimating these integrals one arrives at the leading contribution (for large  $\lambda_0$ )

$$\begin{aligned}
 & 2\lambda_0^2\mu \int (\nabla\phi_0)^2 + \iint \left( \mu\mathbf{p}^2 + 2\lambda_0^2\phi_0(\mathbf{u})^2 \frac{4\pi}{\mathbf{p}^2} \right) f(\mathbf{u}, |\mathbf{p}|) \\
 & \quad - \frac{4\pi}{\mathbf{p}^2} 2\lambda_0^2\phi_0(\mathbf{u})^2 \sqrt{f(\mathbf{u}, |\mathbf{p}|)(f(\mathbf{u}, |\mathbf{p}|) + 1)} \, d\mathbf{p}d\mathbf{u} \\
 & \quad = 2\lambda_0^2\mu \int (\nabla\phi_0)^2 - I_0 \int (2\lambda_0^2)^{5/4} \phi_0^{5/2}, \quad (9.54)
 \end{aligned}$$

where  $I_0$  is as in Theorem 9.2.

If we choose  $\lambda_0 = \sqrt{N/2}$  we get after a simple rescaling that the energy above is  $N^{7/5}$  times the right side of (9.7) (recall that  $\Phi$  was chosen as the minimizer). We also note that the expected number of particles is

$$2\lambda_0^2 + \text{Tr}(\gamma) = N + O(N^{3/5}), \quad (9.55)$$

as  $N \rightarrow \infty$ .

The only remaining problem is to show how a similar energy could be achieved with a wave function with a fixed number of particles  $N$ , i.e., how to show that we really have an upper bound on  $E_0^{(2)}(N)$ . We indicate this fairly simple argument here.

We construct a trial function  $\Psi'$  as above, but with an expected particle number  $N'$  chosen appropriately close to, but slightly smaller than  $N$ . More precisely,  $N'$  will be smaller than  $N$  by an appropriate lower order correction. It is easy to see then that the mean deviation of the particle number distribution in the state  $\Psi'$  is lower order than  $N$ . In fact, it is of order  $\sqrt{N'} \sim \sqrt{N}$ . Using that we have a good lower bound on the energy  $E_0^{(2)}(n)$  for all  $n$  and that  $\Psi'$  is sharply localized around its mean particle number, we may, without changing the energy expectation significantly, replace  $\Psi'$  by a normalized wave function  $\Psi$  that only has particle numbers less than  $N$ . Since the function  $n \mapsto E_0^{(2)}(n)$  is a decreasing function we see that the energy expectation in the state  $\Psi$  is, in fact, an upper bound to  $E_0^{(2)}(N)$ .

### The Upper Bound for the One-component Gas

The upper bound for the one-component gas is proved in a very similar way as for the two-component gas. We shall simply indicate the main differences here. We will again choose a trial state without a fixed particle number, i.e., a grand canonical trial state. Since we know that the one-component gas has a thermodynamic limit and that there is equivalence of ensembles [50], it makes no difference whether we choose a canonical or grand-canonical trial state.

For the state  $\phi_0$  we now choose a normalized function with compact support in  $\Lambda$ , that is constant on the set  $\{x \in \Lambda \mid \text{dist}(x, \partial\Lambda) > r\}$ . We shall choose  $r > 0$  to go to zero as  $L \rightarrow \infty$ . Let us also choose the constant  $n$  such that  $n\phi_0^2 = \rho$  on the set where  $\phi_0$  is constant. Then  $n \approx \rho L^3$ .

Let again  $\phi_\alpha$ ,  $\alpha = 1, \dots$  be an orthonormal family of real functions orthogonal to  $\phi_0$ . As our trial state we choose, this time,

$$\Psi = \prod_{\alpha \neq 0} (1 - \lambda_\alpha^2)^{1/4} \exp\left(-\lambda_0^2/2 + \lambda_0 a_0^* - \sum_{\alpha \neq 0} \frac{\lambda_\alpha}{2} a_\alpha^* a_\alpha^*\right) |0\rangle, \quad (9.56)$$

where  $a_\alpha^*$  is the creation of a particle in the state  $\phi_\alpha$ . We will choose  $\Psi$  implicitly by choosing the operator  $\gamma$  defined as in (9.47).

This time we obtain

$$\begin{aligned} \left(\Psi, \sum_{N=0}^{\infty} H_N^{(1)} \Psi\right) &= \lambda_0^2 \mu \int (\nabla \phi_0)^2 \\ &+ \frac{1}{2} \iint \frac{|\gamma(\mathbf{x}, \mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} dx dy + \frac{1}{2} \iint \frac{|\sqrt{\gamma(\gamma+1)}(\mathbf{x}, \mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} dx dy \\ &+ \frac{1}{2} \iint_{\Lambda \times \Lambda} \frac{(\rho - \rho_\gamma(\mathbf{x}) - \lambda_0^2 \phi_0(\mathbf{x})^2) (\rho - \rho_\gamma(\mathbf{y}) - \lambda_0^2 \phi_0(\mathbf{y})^2)}{|\mathbf{x} - \mathbf{y}|} dx dy \\ &+ \text{Tr}(-\mu \Delta \gamma) + \lambda_0^2 \text{Tr}\left(\mathcal{K}\left(\gamma - \sqrt{\gamma(\gamma+1)}\right)\right), \end{aligned} \quad (9.57)$$

where  $\rho_\gamma(\mathbf{x}) = \gamma(\mathbf{x}, \mathbf{x})$  and  $\mathcal{K}$  is again given as in (9.49). We must show that we can make choices such that the first four terms on the right side above are lower order than the energy, and can therefore be neglected.

We choose

$$\gamma = \gamma_\varepsilon = (2\pi)^{-3} \int_{|p| > \varepsilon \rho^{1/4}} f(|\mathbf{p}|) \mathcal{P}_{\phi_0}^\perp |\theta_{\mathbf{p}}\rangle \langle \theta_{\mathbf{p}}| \mathcal{P}_{\phi_0}^\perp d\mathbf{p}, \quad (9.58)$$

where  $\varepsilon > 0$  is a parameter which we will let tend to 0 at the end of the calculation. Here  $\mathcal{P}_{\phi_0}^\perp$  as before is the projection orthogonal to  $\phi_0$  and this time

$$f(|\mathbf{p}|) = \frac{1}{2} \left( \frac{\mathbf{p}^4 + 8\pi\mu^{-1}\rho}{\mathbf{p}^2 (\mathbf{p}^4 + 16\pi\mu^{-1}\rho)^{1/2}} - 1 \right) \quad (9.59)$$

and

$$\theta_{\mathbf{p}}(x) = \sqrt{n\rho^{-1}} \exp(i\mathbf{p} \cdot \mathbf{x}) \phi_0(\mathbf{x}). \quad (9.60)$$

Note that  $n\rho^{-1}\phi_0(\mathbf{x})^2$  is 1 on most of  $\Lambda$ . We then again have the Berezin–Lieb inequality as before. We also find that

$$\begin{aligned} \rho_\gamma(\mathbf{x}) &= (2\pi)^{-3} \int_{|p| > \varepsilon \rho^{1/4}} f(|\mathbf{p}|) d\mathbf{p} n\rho^{-1} \phi_0(\mathbf{x})^2 \left(1 + O(\varepsilon^{-1} \rho^{-1/4} L^{-1})\right) \\ &= A_\varepsilon (\rho/\mu)^{3/4} n\rho^{-1} \phi_0(\mathbf{x})^2 \left(1 + O(\varepsilon^{-1} \rho^{-1/4} L^{-1})\right), \end{aligned} \quad (9.61)$$

where  $A_\varepsilon$  is an explicit function of  $\varepsilon$ . We now choose  $\lambda_0$  such that  $\lambda_0^2 = n(1 - A_\varepsilon \rho^{-1/4} \mu^{-3/4})$ , i.e., such that

$$\lambda_0^2 \phi_0^2(\mathbf{x}) + \rho_\gamma(\mathbf{x}) = n\phi_0(\mathbf{x})^2 (1 + O(\varepsilon^{-1} \rho^{-1/2} L^{-1})) \approx \rho. \quad (9.62)$$

It is easy to see that the first term in (9.57) is of order  $\rho L^3(rL)^{-1}$  and the fourth term in (9.57) is of order  $\rho L^3(\varepsilon^{-2} + \rho r^2)$ . We may choose  $r$ , depending on  $L$ , in such a way that after dividing by  $\rho L^3$  and letting  $L \rightarrow \infty$  only the error  $\varepsilon^{-2}$  remains. This allows choosing  $\varepsilon \ll \rho^{-1/8}$ .

To estimate the second term in (9.57) we use Hardy's inequality to deduce

$$\iint \frac{|\gamma(\mathbf{x}, \mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} \leq 2(\text{Tr } \gamma^2)^{1/2} \text{Tr } (-\Delta \gamma^2)^{1/2}, \quad (9.63)$$

and these terms can be easily estimated using the Berezin–Lieb inequality in the direction opposite from before, since we are interested now in an upper bound. The third term in (9.57) is controlled in exactly the same way as the second term. We are then left with the last two terms in (9.57). They are treated in exactly the same way as for the two-component gas again using the Berezin–Lieb inequality.

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