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by

H.D. Cornean, J. Dereziński and P. Ziń

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Department of Mathematical Sciences
Aalborg University
Fredrik Bajers Vej 7 G ▪ DK - 9220 Aalborg Øst ▪ Denmark
Phone: +45 96 35 80 80 ▪ Telefax: +45 98 15 81 29
URL: http://www.math.aau.dk

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ON THE INFIMUM OF THE ENERGY-MOMENTUM SPECTRUM OF A HOMOGENEOUS BOSE GAS

H.D. CORNEAN, J. DEREZIŃSKI, AND P. ZIŃ

Abstract. We consider second quantized homogeneous Bose gas in a large cubic box with periodic boundary conditions, at zero temperature, and in the grand canonical setting (the chemical potential μ is fixed, the number of particles can vary). We investigate upper bounds on the infimum of the energy for a fixed total momentum $\mathbf{k}$ given by the expectation value at one-particle excitations over a squeezed state. We show that the results of the Bogoliubov approach (usually derived heuristically) coincide with the results of the first iteration of our method (which leads to rigorous upper bounds).

Contents

1. Introduction

One can distinguish two possible approaches to the Bose gas at density ρ: "canonical" and "grand-canonical". Further on in our paper we will concentrate on the latter setting. Nevertheless, in the introduction, let us stick to the canonical approach.

Suppose that the 2-body potential of an interacting Bose gas is described by a real function v defined on $\mathbb{R}^d$, satisfying $v(\mathbf{x}) = v(-\mathbf{x})$. We assume that $v(x)$ decays at infinity sufficiently fast.

A typical assumption on the potentials that we have in mind in our paper is

$$\hat{v}(\mathbf{k}) > 0, \quad \mathbf{k} \in \mathbb{R}^d, \tag{1.1}$$

where the Fourier transform of v is given by

$$\hat{v}(\mathbf{k}) := \int v(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{x}}\, \mathrm{d}\mathbf{k}. \tag{1.2}$$

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Potentials satisfying (1.1) will be called repulsive. Note, however, that a large part of our paper does not directly use any specific assumption on the potentials.

In order to define the quantities at nonzero density, we start with a system of n bosonic particles in $\Lambda = [0, L]^d$ – the d-dimensional cubic box of side length L. We assume that the number of particles equals $n = \rho V$, where $V = L^d$ is the volume of the box. Following the accepted (although somewhat unphysical) tradition we replace the potential by

$$v^L(\mathbf{x}) = \frac{1}{V} \sum_{\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\, \hat{v}(\mathbf{k}), \tag{1.3}$$

where $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ is the discrete momentum variable. Note that v^L is periodic with respect to the domain Λ, and $v^L(\mathbf{x}) \to v(\mathbf{x})$ as $L \to \infty$. The system in a box is described by the Hamiltonian

$$H^{L,n} = -\sum_{i=1} \frac{1}{2}\Delta_i + \sum_{1 \le i < j \le n} v^L(\mathbf{x}_i - \mathbf{x}_j) \tag{1.4}$$

acting on the space $L^2_{\mathrm{s}}(\Lambda^n)$ (symmetric square integrable functions on Λ^n). We assume that the Laplacian has periodic boundary conditions.

Let us denote by $E^{L,n}$ the *ground state energy in the box:*

$$E^{L,n} := \inf \mathrm{sp} H^{L,n},$$

where $\mathrm{sp}K$ denotes the spectrum of an operator K.

The total momentum is given by the operator

$$P^{L,n} := \sum_{i=1}^{n} -\mathrm{i}\nabla_{\mathbf{x}_i}.$$

Its spectrum equals $\frac{2\pi}{L}\mathbb{Z}^d$.

Note that $H^{L,n}$ and $P^{L,n}$ commute with each other. Therefore we can define the joint spectrum of these operators

$$\mathrm{sp}(H^{L,n}, P^{L,n}) \subset \mathbb{R} \times \frac{2\pi}{L}\mathbb{Z}^d,$$

which will be called the *energy-momentum spectrum in the box.* For $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$, we define the *infimum of the energy-momentum spectrum in the box* to be

$$\inf\{s \ : \ (s, \mathbf{k}_L) \in \mathrm{sp}(H^{L,n}, P^{L,n})\}. \tag{1.5}$$

The main subject of our paper is studying upper bounds to (1.5).

We would also like to use this paper as an occasion to state precisely some conjectures about the energy-momentum spectrum of Bose gas with repulsive interactions in themodynamical limit. These conjectures are suggested by various heuristic arguments, notably due to Bogoliubov. They go far beyond what we can prove rigorously at the moment.

By the *excitation spectrum in the box* we will mean $\mathrm{sp}(H^{L,n} - E^{L,n}, P^{L,n})$. For $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$, we define the *infimum of the excitation spectrum (IES) in the box* as

$$\epsilon^{L,n}(\mathbf{k}_L) := \inf\{s \ : \ (s, \mathbf{k}_L) \in \mathrm{sp}(H^{L,n}, P^{L,n})\} - E^{L,n}. \tag{1.6}$$

Let $L \to \infty$ with $\rho = \frac{n}{L^d}$. The momentum lattice $\frac{2\pi}{L}\mathbb{Z}^d$ converges in some sense to the continuous space $\mathbb{R}^d$. The Hamiltonians $H^{L,n} - E^{L,n}$ do not have a limit in any meaning known to us. Nevertheless, we would like to define the IES in this limit as a function on $\mathbb{R}^d$. It is not obvious how to do it. We propose the following definition:

For $\mathbf{k} \in \mathbb{R}^d$ and $\rho > 0$, we take $\delta > 0$ and set

$$\epsilon^\rho(\mathbf{k}, \delta) \quad := \quad \liminf_{n\to\infty} \left(\inf \left\{ \epsilon^{L,n}(\mathbf{k}'_L) \ : \ \mathbf{k}'_L \in \frac{2\pi}{L}\mathbb{Z}^d, \ |\mathbf{k} - \mathbf{k}'_L| < \delta, \ \rho = \frac{n}{L^d} \right\} \right).$$

This gives a lower bound on the IES for the momenta $\mathbf{k}_L$ in the window in the momentum space around $\mathbf{k}$ of diameter 2δ. The quantity $\epsilon^\rho(\mathbf{k}, \delta)$ increases as δ becomes smaller. The *IES at the thermodynamic limit* is defined as its supremum (or, equivalently, its limit) as $\delta \searrow 0$:

$$\epsilon^\rho(\mathbf{k}) := \sup_{\delta > 0} \epsilon^\rho(\mathbf{k}, \delta).$$

Under Assumption (1.1) it is easy to prove that $E^{L,n}$ is finite and $\epsilon^{L,n}(0) = \epsilon^\rho(0) = 0$ (see Theorem 4.1 and Proposition 4.2).

Conjecture 1.1. We expect that for a large class of repulsive potentials the following statements hold true:

(1) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon^\rho(\mathbf{k}) \in \mathbb{R}_+$ is continuous.
(2) Let $\mathbf{k} \in \mathbb{R}^d$. If $\{L_s\}_{s\geq 1} \subset \mathbb{R}$ diverges to $+\infty$, and $\rho = n_s/L_s^d$, then for every sequence $\mathbf{k}_s \in \frac{2\pi}{L_s}\mathbb{Z}^d$ which obeys $\mathbf{k}_s \to \mathbf{k}$, we have that $\epsilon^{L_s,n_s}(\mathbf{k}_s) \to \epsilon(\mathbf{k})$.
(3) If $d \geq 2$, then $\inf_{\mathbf{k}\neq 0} \frac{\epsilon(\mathbf{k})}{|\mathbf{k}|} =: c_{\mathrm{cr}} > 0$.
(4) There exists $c_{\mathrm{s}} > 0$ such that $\lim_{\mathbf{k}\to 0} \frac{\epsilon(\mathbf{k})}{|\mathbf{k}|} = c_{\mathrm{s}}$.

Statements (1) and (2) can be interpreted as some kind of a "spectral thermodynamic limit in the canonical approach". Note that if (1) and (2) are true around $\mathbf{k} = 0$, then we can say that there is "no gap in the excitation spectrum".

The properties (3) and (4) of the Bose gas were predicted by Landau in the 40's. Shortly thereafter, they were derived by a somewhat heuristic argument by Bogoliubov [2]. They seem to have been confirmed experimentally (see e.g. [13]).

(3) is commonly believed to be responsible for the superfluidity of the Bose gas. More precisely, it is argued that because of (3) a drop of Bose gas travelling at speed less than c_{cr} will experience no friction.

(4) implies that the sound has a well defined speed at low frequencies equal to c_{s}.

Note that in dimension $d = 1$ the condition (3) should be replaced by

(3)' If $d = 1$, then $\epsilon^\rho(\mathbf{k} + 2\pi\rho) = \epsilon^\rho$.

The statement (3)' has a simple rigorous proof, which we will give later on in our paper. It implies that in dimension $d = 1$ the excitation spectrum is periodic with the period $2\pi\rho$.

The original argument of Bogoliubov is based on the idea that in thermodynamical limit homogeneous Bose gas with repulsive interactions can be effectively described by a quadratic bosonic Hamiltonian. For quadratic Hamiltonians one can easily find the infimum of the excitation spectrum. For instance, for the free Bose gas the IES is not very interesting: it just equals zero for all momenta. However, there exist quadratic Hamiltonians with the IES of the form described by (3) or (3)', and (4). One can argue that this fact indicates that Conjectures 1.1 and 4.3 are plausible. We describe some relevant facts about the energy-momentum spectra of quadratic Hamiltonians in Appendix A. We could not find these facts in the literature, although they probably belong to the folk knowledge.

To our experience, most physicists interested in this subject (but not all) would agree that one should expect Conjecture 1.1 (as well as the analogous Conjecture 4.3 formulated in the grand-canonical setting) to be true. To our surprise, in the literature devoted to this subject the authors seem to avoid making precise conjectures about these things. In particular, we have not seen a rigorous definition of the IES similar to (1.7).

Since Bogoliubov, many theoreticians have worked on this subject. Nevertheless, to our knowledge, no satisfactory rigorous analysis of the energy-momentum spectrum of the Bose gas exists. Only in the one-dimensional case, when the interaction v is a repulsive delta-function, it can be described fairly explicitly (see [9, 8]) and at least one can prove that there is no gap in it in the thermodynamical limit.

Almost all theoretical works on the energy-momentum spectrum of the Bose gas instead of the correct Hamiltonian $H^{L,n}$ (or its second-quantized version H^L and the grand-canonical version H_μ^L) considered its modifications. They either replaced the zero mode by a c-number or dropped some of the terms, or did both modifications [1, 7, 5, 6, 15, 16]. These Hamiltonians have no independent physical justification apart from being approximations to the correct Hamiltonian in some uncontrolled way.

In our paper we are not interested in any such modified Hamiltonians: all our statements will be related to the grand-canonical Hamiltonian H_μ^L (the natural second quantization of $H^{L,n} - \mu n$). Note however, that some of the quantities we study are not quite the ones we are interested in: instead of the bottom of the spectrum, most of the time we consider its upper bounds given by the expectation values between some restricted classes of vectors.

In many papers on the Bose gas one does not obtain a cusp at the bottom of the excitation spectrum. One usually obtains a small gap between the ground state energy and the lowest excitation. There is no such gap in the calculations of Bogoliubov, as crude as they are. However, when one tries to "improve" on Bogoliubov's calculations, the gap usually appears. Yet, there are arguments that this gap is an artifact of these approximations, and in the complete treatment it should not appear, see Hugenholtz-Pines [7], Girardeau-Nozieres [5], and the $\frac{1}{q^2}$ Theorem of Bogoliubov [3]. To our understanding, these arguments are not yet complete proofs of a statement similar to Conjectures 1.1 and 4.3. We believe that to prove or disprove them would be an interesting subject for research in mathematical physics.

One should remark that there exists a large rigorous literature on the Bose gas, see e.g. [10] or the recent lecture notes of Lieb, Seiringer, Solovej and Yngvason [11] and references therein. This literature, however, is devoted mostly to the study of the ground state energy or the pressure, and not to the dependence of the infimum of the excitation spectrum on momentum.

The main purpose of our paper is to describe two methods that can be used to give upper bounds on the infimum of the energy-momentum spectrum. The first, which we call the Squeezed States Approximation (SSA), uses squeezed states and 1-particle excitations over squeezed states to obtain a variational estimate. The second, which we call the Improved Bogoliubov Approximation (IBA) is a modification of the SSA, and gives a less precise estimate. These methods leads to functions $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon_{\mathrm{ssa},\mu}(\mathbf{k})$, $\epsilon_{\mathrm{iba},\mu}(\mathbf{k})$, which can be viewed as the approximation to the true IES $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon_\mu(\mathbf{k})$ in SSA and IBA respectively.

By squeezed states we mean states obtained from the vacuum by a Bogoliubov translation and rotation. Note that the requirement of the translation symmetry restricts the choice of these transformations. In particular, only a translation of the zero mode is allowed and only pairs of particles of opposite momenta can be created.

To our knowledge, in the context of the Bose gas, the idea of using squeezed states to bound the ground state energy first appeared in the paper of Robinson [14]. Robinson considered a slightly more general class of states – quasi-free states.

He noticed, however, that in the case he looked at it is sufficient to restrict to pure quasi-free states – which coincide with squeezed states. One should mention also [4], where a variational bound on the pressure of Bose gas in a positive temperature is derived by using quasi-free states.

Only an upper bound to the ground state energy is considered in [14]. We go one step further: we show how this method can be extended to obtain upper bounds on the infimum of the energy-momentum spectrum by using one-particle excitations over squeezed states.

The method IBA seems to be much more convenient computationally then SSA. We show that it leads to a relatively simple fixed point equation, which can be used to obtain the upper bounds. It seems that the quantities involved in IBA have limits as $L \to \infty$. This is at least suggested by formal arguments. It would be interesting to rigorously prove that this is true.

Note that the method IBA seems also well suited as the first step to a systematic perturbative treatment of the Bose gas. It leads to the construction of an effective Hamiltonian, which can serve as the main part of the full Hamiltonian H_μ^L, whereas the reminder can be treated as a perturbation.

Clearly, the function $\epsilon_{\mathrm{iba},\mu}(\mathbf{k})$ has a well defined physical meaning for a finite volume: added to the ground state energy it gives an upper bound on the infimum of the energy-momentum spectrum. In the thermodynamical limit this loses its validity, since the infimum of the energy-momentum spectrum in the grand-canonical approach seems to go to $-\infty$. However, following the experience of many similar physical theories, we hope that the approximations we introduced are somehow close to reality. In other words, we would not be surprised if $\epsilon_{\mathrm{iba},\mu}(\mathbf{k})$ turned out to be close to $\epsilon_\mu(\mathbf{k})$. If under some conditions this is true, it would be interesting to describe and justify this closeness rigorously.

There exists a natural iterative procedure that one can try to use in order to solve the fixed point equation of IBA. The first iteration of this procedure gives a result which coincides with the original Bogoliubov approximation in its grand-canonical version. This explains why both approximations look so similarly. In particular, in both IBA and Bogoliubov's calculations, one has a step which amounts to replacing the zero mode by a c-number, and one performs a Bogoliubov rotation. However, whereas IBA has a clear rigorous meaning (it gives an upper bound), Bogoliubov's calculations are presentedpurely heuristic.

As we discussed above, the repulsive Bose gas in dimension $d = 1$ has a periodic IES. Therefore, it is clear that the methods SSA and IBA give poor upper bounds in $d = 1$ for large momenta.

Actually, our hope that the methods SSA and IBA give answers close to reality has another weak point in any dimension d. Equation (10.11) indicates that $\epsilon_{\mathrm{iba},\mu}(\mathbf{k})$ has a nonzero gap, at least if IBA involves a nontrivial Bogoliubov rotation and traslation, and if the infinite volume limit can be justified. Therefore, it seems that IBA does not give the correct qualitative shape of the true IES.

Perhaps, this is the most important (even if negative) finding of our paper. It implies that at the bottom of its spectrum, repulsive Bose gas should be approximated by a more complicated ansatz, than just what we propose. In the literature, the existence of a gap in various approximation schemes, which try to improve on the original Bogoliubov's one, has been noticed by a number of authors [6, 15]. However, to our knowledge these authors did not consider the correct Hamiltonian, but always used one of its distorted versions.

The structure of our paper is as follows:

In Section 2 we recall the original Bogoliubov calculations. They use the canonical approach.

In Section 3 we discuss the case of dimension $d = 1$.

In Section 4 we introduce the notation in the grand-canonical setting. We state a conjecture analogous to Conecture 1.1 in this setting. The grand-canonical approach is used throughout the later part of the paper as well.

In Section 5 we describe the original Bogoliubov calculations adapted to the grand-canonical approach.

Sections 2, 3 and 5 should be viewed as an extension of the introduction, included for a historical perspective and for comparison with the results obtained in later sections.

The main part of our paper starts with Section 6 where we describe the Squeezed States Approximation. In Section 7 we describe the Improved Bogoliubov Approximation.

In Sections 8 and 9 we derive the basic fixed point equation for the Improved Bogoliubov Approximation. It is described in Theorem 10.1.

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2. Original Bogoliubov approach

As realized by Bogoliubov, even if one is interested in properties of the Bose gas with a fixed but large number of particles, it is convenient to pass to the second quantized description of the system, allowing an arbitrary number of particles. To this end one introduces the second quantized form of (1.4), that is

$$\begin{aligned} H^L &= -\int a_{\mathbf{x}}^* \frac{1}{2}\Delta_{\mathbf{x}} a_{\mathbf{x}} \mathrm{d}\mathbf{x} \\ &\quad +\frac{1}{2}\int\int a_{\mathbf{x}}^* a_{\mathbf{y}}^* v^L(\mathbf{x}-\mathbf{y}) a_{\mathbf{y}} a_{\mathbf{x}} \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}, \end{aligned} \tag{2.1}$$

acting on the symmetric Fock space $\Gamma_{\mathrm{s}}(L^2(\Lambda))$. It is convenient to pass to the momentum representation:

$$\begin{aligned} H^L = &\sum_{\mathbf{k}} \frac{1}{2}\mathbf{k}^2 a_{\mathbf{k}}^* a_{\mathbf{k}} \qquad (2.2) \\ &+ \frac{1}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\hat{v}(\mathbf{k}_2-\mathbf{k}_3) a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}, \end{aligned}$$

where we used (1.3) to replace $v^L(\mathbf{x})$ with the Fourier coefficients $\hat{v}(\mathbf{k})$. Note that $\hat{v}(\mathbf{k}) = \hat{v}(-\mathbf{k})$, and $a_{\mathbf{x}} = V^{-1/2}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}} a_{\mathbf{k}}$.

Recall that the number and momentum operator are defined as

$$N^L := \sum_{\mathbf{k}} a_{\mathbf{k}}^* a_{\mathbf{k}}, \quad P^L := \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^* a_{\mathbf{k}}. \tag{2.3}$$

$H^{L,n}$ and $P^{L,n}$ coincide with the operators H^L and P^L restricted to the eigenspace of N^L with the eigenvalue n.

Let us proceed following the original method of Bogoliubov. We make an ansatz consisting in replacing the operators a_0^*, a_0 with c-numbers:

$$a_0^* a_0 \approx |\alpha|^2, \quad a_0 \approx \alpha, \quad a_0^* \approx \overline{\alpha}. \tag{2.4}$$

We drop higher order terms. We will write $\sum_{\mathbf{k}}'$ for $\sum_{\mathbf{k}\neq 0}$.

$$\begin{aligned} H^L \quad \approx \quad & \sum_{\mathbf{k}}{}' \left(\frac{1}{2}\mathbf{k}^2 + \frac{\hat{v}(0)+\hat{v}(\mathbf{k})}{V}|\alpha|^2\right) a_{\mathbf{k}}^* a_{\mathbf{k}} \\ & + \sum_{\mathbf{k}}{}' \left(\frac{\hat{v}(\mathbf{k})\alpha^2}{2V} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + \frac{\hat{v}(\mathbf{k})\overline{\alpha}^2}{2V} a_{\mathbf{k}} a_{-\mathbf{k}}\right) + \frac{\hat{v}(0)}{2V}|\alpha|^4. \end{aligned} \tag{2.5}$$

Then we replace α with ρ, setting

$$|\alpha|^2 + \sum_{\mathbf{k}}{}' a_{\mathbf{k}}^* a_{\mathbf{k}} = \rho V,$$

and again we drop the higher order terms. Thus for $n \approx \rho V$ we obtain

$$\begin{aligned} H^{L,n} \approx \quad H_{\mathrm{bg}}^{L,\rho} := \quad & \sum_{\mathbf{k}}{}' \left(\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\rho\right) a_{\mathbf{k}}^* a_{\mathbf{k}} \\ & + \sum_{\mathbf{k}}{}' \frac{\hat{v}(\mathbf{k})\rho}{2} \left(\frac{\alpha^2}{|\alpha|^2} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + \frac{\overline{\alpha}^2}{|\alpha|^2} a_{\mathbf{k}} a_{-\mathbf{k}}\right) + \frac{\hat{v}(0)}{2} V\rho^2. \end{aligned}$$

We perform the Bogoliubov rotation to separate the Hamiltonian into normal modes:

$$a_{\mathbf{k}}^* = c_{\mathbf{k}} b_{\mathbf{k}}^* - s_{\mathbf{k}} b_{-\mathbf{k}}, \quad a_{\mathbf{k}} = c_{\mathbf{k}} b_{\mathbf{k}} - s_{\mathbf{k}} b_{-\mathbf{k}}^*,$$

where

$$s_{\mathbf{k}} \quad = \quad \frac{\alpha}{\sqrt{2}|\alpha|} \left(\left(1 - \left(\frac{\rho\hat{v}(\mathbf{k})}{\frac{1}{2}\mathbf{k}^2 + \rho\hat{v}(\mathbf{k})}\right)^2\right)^{-1/2} - 1 \right)^{1/2}. \tag{2.6}$$

and $c_{\mathbf{k}} = \sqrt{1 + |s_{\mathbf{k}}|^2}$. We obtain

$$H_{\mathrm{bg}}^{L,\rho} \quad = \quad \sum_{\mathbf{k}}{}' \omega_{\mathrm{bg}}^{\rho}(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}} + E_{\mathrm{bg}}^{L,\rho}, \tag{2.7}$$

where the elementary excitation spectrum of H_{bg}^{ρ} is

$$\omega_{\mathrm{bg}}^{\rho}(\mathbf{k}) = \sqrt{\frac{1}{2}\mathbf{k}^2 (\frac{1}{2}\mathbf{k}^2 + 2\hat{v}(\mathbf{k})\rho)}, \tag{2.8}$$

and its ground state energy equals

$$\begin{aligned} E_{\mathrm{bg}}^{L,\rho} \quad = \quad & \frac{\hat{v}(0)}{2} V\rho^2 \\ & + \sum_{\mathbf{k}}{}' \frac{1}{2}\left(\omega_{\mathrm{bg}}(\mathbf{k}) - (\frac{1}{2}\mathbf{k}^2 + \rho\hat{v}(\mathbf{k}))\right). \end{aligned} \tag{2.9}$$

Now, as discussed in Appendix A, the IES of $H_{\mathrm{bg}}^{L,\rho}$ is given by

$$\epsilon_{\mathrm{bg}}^{\rho}(\mathbf{k}) = \inf\{\omega_{\mathrm{bg}}^{\rho}(\mathbf{k}_1) + \cdots + \omega_{\mathrm{bg}}^{\rho}(\mathbf{k}_n) \ : \ \mathbf{k}_1 + \cdots + \mathbf{k}_n = \mathbf{k}, \quad n = 1, 2, \dots\}.$$

Note that (in any dimension)

(1) $\inf_{\mathbf{k}\neq 0} \frac{\omega_{\mathrm{bg}}^{\rho}(\mathbf{k})}{|\mathbf{k}|} = c_{\mathrm{cr}} > 0$;

(2) $\lim_{\mathbf{k}\to 0} \frac{\omega_{\mathrm{bg}}^{\rho}(\mathbf{k})}{|\mathbf{k}|} = c_{\mathrm{s}}$.

with $c_{\mathrm{cr}} := \inf \sqrt{\frac{1}{2}(\frac{1}{2}\mathbf{k}^2 + 2\hat{v}(\mathbf{k})\rho)}$ and $c_{\mathrm{s}} := \sqrt{\rho\hat{v}(0)}$. Therefore, by Theorem A.4 (1) and (2) we have

(1) $\inf_{\mathbf{k}\neq 0}\frac{\epsilon_{\mathrm{bg}}^{\rho}(\mathbf{k})}{|\mathbf{k}|}=c_{\mathrm{cr}}$;

(2) $\lim_{\mathbf{k}\to 0}\frac{\epsilon_{\mathrm{bg}}^{\rho}(\mathbf{k})}{|\mathbf{k}|}=c_{\mathrm{s}}$.

Thus, the IES of $H_{\mathrm{bg}}^{L,\rho}$ has all the properties described in Conjecture 1.1.

We can also compute that for small $|\mathbf{k}|$

$$s_{\mathbf{k}}\approx\frac{\alpha}{\sqrt{2}|\alpha|}\left(\rho\hat{v}(0)\right)^{1/4}|\mathbf{k}|^{-1/2}. \tag{2.10}$$

Therefore, if Ψ denotes the ground state of (2.9), then

$$(\Psi|a_{\mathbf{k}}^{*}a_{\mathbf{k}}\Psi)=|s_{\mathbf{k}}|^{2}\approx\frac{\left(\rho\hat{v}(0)\right)^{1/2}}{2|\mathbf{k}|}.$$

The density of particles ρ equals

$$\frac{|\alpha|^{2}}{V}+\frac{1}{V}\sum_{\mathbf{k}}{}^{\prime}|s_{\mathbf{k}}|^{2}. \tag{2.11}$$

We expect that for large L, (2.11) converges to

$$\rho_{0}+\frac{1}{(2\pi)^{d}}\int|s_{\mathbf{k}}|^{2}\mathrm{d}\mathbf{k}. \tag{2.12}$$

3. Bose gas in dimension $d=1$

Bosonic gas in dimension $d=1$ seems to have different properties than in higher dimensions. In particular, statement (3) of Conjecture 1.1 should be replaced by (3)'.

Let us prove the statement (3)'. Consider first the system of n bosons in an interval of size L, with $\rho=\frac{n}{L}$. For any $m\in\mathbb{Z}$, define the operator

$$U:=\exp\left(\frac{\mathrm{i}2\pi}{L}\sum_{i=1}^{n}\mathbf{x}_{i}\right).$$

Clearly, U is a unitary operator on $L_{\mathrm{s}}(\mathbb{R}^{n})$ satisfying

$$\begin{aligned}U^{*}P^{L,n}U&=P^{L,n}+2\pi\rho,\\ U^{*}H^{L,n}U&=H^{L,n}-\frac{2\pi}{L}P^{L,n}+\frac{(2\pi)^{2}}{2L}\rho.\end{aligned}$$

Hence if Φ is a common eigenvector of the Hamiltonian and the momentum with

$$\begin{aligned}(H^{L,n}-E)\Phi&=0,\\ (P^{L,n}-\mathbf{k})\Phi&=0,\end{aligned}$$

then

$$\begin{aligned}(H^{L,n}-E)U\Phi&=\frac{1}{L}(-2\pi\mathbf{k}+2\pi^{2}\rho)U\Phi,\\ (P^{L,n}-\mathbf{k}-2\pi\rho)U\Phi&=0,\end{aligned}$$

Considering $L\to\infty$, we see that the IES in thermodynamical limit is periodic in $\mathbf{k}$ with the period equal to $2\pi\rho$.

Another peculiarity of dimension $d=1$ is related to the formula (2.12). We note that $|\mathbf{k}|^{-1}$ is integrable only in dimension $d>1$. Therefore, for $d=1$ (2.12) diverges. Thus, the Bogoliubov approximation is problematic for $d=1$ if we keep the density ρ fixed as $L\to\infty$. To our knowledge, (2.10) and the above described problem of the Bogoliubov approximation in $d=1$ was first noticed in [5].

Nevertheless, in spite of the breakdown of the Bogoliubov approximation, many authors believe that the IES in $d=1$ exhibits the behavior $\epsilon^{\rho}(\mathbf{k})\approx c_{\mathrm{s}}(\mathbf{k})$ for low momenta, see e.g. [12], Chapter 6.

4. Grand-canonical approach to the Bose gas

It was noted already by Beliaev [1], Hugenholz - Pines [7] and others that instead of studying the Bose gas in the canonical formalism, fixing the density, it is more mathematically convenient to use the grand-canonical formalism and fix the chemical potential. Then one can pass from the chemical potential to the density by the Legendre transformation.

More precisely, for a given chemical potential $\mu > 0$, we define the grand-canonical Hamiltonian

$$\begin{aligned} H_\mu^L &:= H^L - \mu N^L \\ &= \sum_{\mathbf{k}} (\frac{1}{2}\mathbf{k}^2 - \mu) a_{\mathbf{k}}^* a_{\mathbf{k}} \\ &+ \frac{1}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \hat{v}(\mathbf{k}_2 - \mathbf{k}_3) a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}. \end{aligned} \tag{4.1}$$

The ground state energy in the grand-canonical approach is defined as

$$E_\mu^L = \inf \mathrm{sp} H_\mu^L = \inf_{n\geq 1} (E^{L,n} - \mu n). \tag{4.2}$$

Note that the corresponding density ρ is given by

$$\partial_\mu E_\mu^L \quad = \quad -V\rho. \tag{4.3}$$

Both $E^{L,n}$ and E_μ^L are finite for a large class of potentials, which follows from a simple rigorous result, which we state below.

Theorem 4.1. *Suppose that $\hat{v}(\mathbf{k}) \geq 0$, $\hat{v}(0) > 0$ and $v(0) < \infty$. Then $H^{L,n}$ and H_μ^L are bounded from below and*

$$E^{L,n} \quad \geq \quad \frac{\hat{v}(0)}{2V} n^2 - \frac{v(0)}{2} n, \tag{4.4}$$

$$E_\mu^L \quad \geq \quad -V \frac{(\frac{1}{2}v(0) + \mu)^2}{2\hat{v}(0)}. \tag{4.5}$$

For $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$ we define the *IES in the box*

$$\epsilon_\mu^L(\mathbf{k}_L) := \inf\{s \;:\; (s, \mathbf{k}_L) \in \mathrm{sp}(H_\mu^L, P^L)\} - E^L. \tag{4.6}$$

For $\mathbf{k} \in \mathbb{R}^d$ we define the *IES at the thermodynamic limit*

$$\epsilon_\mu(\mathbf{k}) := \sup_{\delta>0} \left(\liminf_{L\to\infty} \left(\inf_{\mathbf{k}'_L \in \frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k}-\mathbf{k}'_L|<\delta} \epsilon_\mu^L(\mathbf{k}'_L) \right) \right). \tag{4.7}$$

Another natural definition would be:

$$\tilde{\epsilon}_\mu(\mathbf{k}) := \inf_{\delta>0} \left(\limsup_{L\to\infty} \left(\sup_{\mathbf{k}'_L \in \frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k}-\mathbf{k}'_L|<\delta} \epsilon_\mu^L(\mathbf{k}'_L) \right) \right). \tag{4.8}$$

This bounds from above the IES in the box in every window of diameter 2δ. Clearly, $\epsilon_\mu(\mathbf{k}) \leq \tilde{\epsilon}(\mathbf{k})$. Although it is not obvious that $\tilde{\epsilon}_\mu$ and ϵ_μ are actually equal, we only consider $\epsilon_\mu(\mathbf{k})$ in this paper.

Now let us formulate some results and conjectures on the behavior of the IES.

Proposition 4.2. *At zero total momentum, the excitation spectrum has a global minimum where it equals zero: $\epsilon^{L,n}(0) = \epsilon^\rho(0) = 0$ and $\epsilon_\mu^L(0) = \epsilon_\mu(0) = 0$.*

Proof. Each $E^{L,n}$ is a non-degenerate eigenvalue of $H^{L,n}$, and $H^{L,n}$ commutes with the total momentum and space inversion. Thus each $E^{L,n}$ corresponds to zero total momentum, and hence by (4.2) so does E^L_μ. Hence $\epsilon^{L,n}(0) = \epsilon^L_\mu(0) = 0$. $\square$

Let us now formulate the conjectures about $\epsilon_\mu(\mathbf{k})$ (analogous to the Conjecture 4.3 about $\epsilon^\rho(\mathbf{k})$):

Conjecture 4.3. We expect the following statements to hold true:

(1) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon_\mu(\mathbf{k}) \in \mathbb{R}_+$ is continuous.
(2) Let $\mathbf{k} \in \mathbb{R}^d$. If $\{L_s\}_{s\geq 1} \subset \mathbb{R}$ diverges to $+\infty$, then for every sequence $\mathbf{k}_s \in \frac{2\pi}{L_s}\mathbb{Z}^d$ which obeys $\mathbf{k}_s \to \mathbf{k}$, we have that $\epsilon^{L_s}_\mu(\mathbf{k}_s) \to \epsilon(\mathbf{k})$.
(3) If $d \geq 2$, then $\inf_{\mathbf{k}\neq 0} \frac{\epsilon(\mathbf{k})}{|\mathbf{k}|} =: c_{\mathrm{cr}} > 0$.
(4) There exists $c_{\mathrm{s}} > 0$ such that $\lim_{\mathbf{k}\to 0} \frac{\epsilon_\mu(\mathbf{k})}{|\mathbf{k}|} = c_{\mathrm{s}}$.

Throughout most of our paper, the chemical potential μ is considered to be the natural parameter of our problem. If we want to pass to canonical conditions (fixed density), then we need to prove that

$$e_\mu := \lim_{L\to\infty} \frac{E^L_\mu}{L^d}$$

exists and defines a differentiable, concave function of μ. Denote by $\mu(\rho)$ the unique solution to the equation $-\partial_\mu e_{\mu(\rho)} = \rho$. Then $\epsilon^\rho(\mathbf{k}) = \epsilon_{\mu(\rho)}(\mathbf{k})$.

5. Grand-canonical version of the original Bogoliubov approach

Let us describe the version of the original Bogoliubov approximation adapted to the grand-canonical approach. We follow e.g. Zagrebnov-Bru [16].

We make the replacement (2.4) and drop higher order terms:

$$\begin{aligned} H^L_\mu \approx \quad H^L_{\mathrm{bg},\mu} := \quad & \sum_{\mathbf{k}}{}' \left(\frac{1}{2}\mathbf{k}^2 - \mu + \frac{\hat{v}(0)+\hat{v}(\mathbf{k})}{V}|\alpha|^2\right) a^*_{\mathbf{k}} a_{\mathbf{k}} \\ & + \sum_{\mathbf{k}}{}' \Big(\frac{\hat{v}(\mathbf{k})\alpha^2}{2V} a^*_{\mathbf{k}} a^*_{-\mathbf{k}} + \frac{\hat{v}(\mathbf{k})\overline{\alpha}^2}{2V} a_{\mathbf{k}} a_{-\mathbf{k}}\Big) \\ & + \frac{\hat{v}(0)}{2V}|\alpha|^4 - \mu V |\alpha|^2. \end{aligned}$$

We perform the Bogoliubov rotation and obtain

$$H^L_{\mathrm{bg},\mu} \quad = \quad \sum_{\mathbf{k}}{}' \omega_{\mathrm{bg},\mu}(\mathbf{k}) b^*_{\mathbf{k}} b_{\mathbf{k}} + E^L_{\mathrm{bg},\mu}, \tag{5.1}$$

where the excitation spectrum is

$$\omega_{\mathrm{bg},\mu}(\mathbf{k}) = \sqrt{\big(\frac{1}{2}\mathbf{k}^2 - \mu + |\alpha|^2 \frac{\hat{v}(0)}{V}\big)\big(\frac{1}{2}\mathbf{k}^2 - \mu + |\alpha|^2 \frac{\hat{v}(0)+2\hat{v}(\mathbf{k})}{V}\big)} \tag{5.2}$$

and the ground state energy equals

$$\begin{aligned} E^L_{\mathrm{bg},\mu} \;=\; & \frac{\hat{v}(0)}{2}\frac{|\alpha|^4}{V} - \mu|\alpha|^2 \\ & + \sum_{\mathbf{k}}{}' \frac{1}{2}\Big(\omega(\mathbf{k}) - \big(\frac{1}{2}\mathbf{k}^2 - \mu + |\alpha|^2 \frac{\hat{v}(0)+\hat{v}(\mathbf{k})}{V}\big)\Big). \end{aligned} \tag{5.3}$$

Note that

$$\omega_{\mathrm{bg},\mu}(\mathbf{k}) - \big(\frac{1}{2}\mathbf{k}^2 - \mu + |\alpha|^2 \frac{\hat{v}(0)+\hat{v}(\mathbf{k})}{V}\big)$$

$$\approx \quad -\frac{1}{2}\left(\frac{1}{2}\mathbf{k}^2 - \mu + |\alpha|^2 \frac{\hat{v}(0)+\hat{v}(\mathbf{k})}{V}\right)^{-1} |\alpha|^4 \frac{\hat{v}(\mathbf{k})^2}{V^2}.$$

Hence the term with $\sum'$ in (5.3) is second order in the interaction. Therefore, keeping only first order terms we obtain

$$E^L_{\mathrm{bg},\mu} \approx \frac{\hat{v}(0)}{2V}|\alpha|^4 - \mu|\alpha|^2.$$

To find the lowest ground state energy for a given μ we compute

$$0 = \partial_{|\alpha|^2} E^L_{\mathrm{bg},\mu} \approx \frac{\hat{v}(0)}{V}|\alpha|^2 - \mu,$$

which gives $\mu \approx \frac{\hat{v}(0)}{V}|\alpha|^2$. Thus

$$E^L_{\mathrm{bg},\mu} \approx -\frac{\hat{v}(0)|\alpha|^4}{2V} = -\frac{\mu^2 V}{2\hat{v}(0)}.$$

Applying (4.3) we obtain $\mu = \rho\hat{v}(0)$. If we insert this into (5.3) and (5.2), we obtain expressions identical to (2.9) and (2.8).

6. Infimum of the excitation spectrum in the squeezed states approximation

In what follows we will always use the grand-canonical approach. We will drop μ from H^L_μ, $\epsilon_\mu(\mathbf{k})$, etc.

In this section we describe an approximate method, which will give a rigorous upper bound on E^L and $E^L + \epsilon^L(\mathbf{k})$. The main idea of this method is the use of the so-called squeezed states. (See Appendix B for a brief summary of basic properties of squeezed states).

Let $\alpha \in \mathbb{C}$ and $\frac{2\pi}{L}\mathbb{Z}^d \ni \mathbf{k} \mapsto \theta_{\mathbf{k}} \in \mathbb{C}$ be a square summable sequence with $\theta_{\mathbf{k}} = \theta_{-\mathbf{k}}$. Set

$$W_\alpha := \mathrm{e}^{-\alpha a_0^* + \overline{\alpha} a_0}, \quad U_\theta := \prod_{\mathbf{k}} \mathrm{e}^{-\frac{1}{2}\theta_{\mathbf{k}} a^*_{\mathbf{k}} a^*_{-\mathbf{k}} + \frac{1}{2}\overline{\theta}_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}}$$

Then $U_{\alpha,\theta} := W_\alpha U_\theta$ is the general form of a Bogoliubov transformation commuting with P^L. Let Ω denote the vacuum vector. Note that

$$\Psi_{\alpha,\theta} := U^*_{\alpha,\theta}\Omega$$

is the general form of a squeezed vector of zero momentum. Vectors of the form

$$\Psi_{\alpha,\theta,\mathbf{k}} := U^*_{\alpha,\theta} a^*_{\mathbf{k}}\Omega$$

are normalized and have momentum $\mathbf{k}$, that means

$$(P^L - \mathbf{k})\Psi_{\alpha,\theta,\mathbf{k}} = 0.$$

By the Squeezed States Approximation (SSA) we will mean applying the variational method using only vectors like $\Psi_{\alpha,\theta}$ and $\Psi_{\alpha,\theta,\mathbf{k}}$.

We define the *SSA ground state energy in the box*

$$E^L_{\mathrm{ssa}} := \inf_{\alpha,\theta}(\Psi_{\alpha,\theta}|H^L\Psi_{\alpha,\theta}).$$

For $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$ we define the *SSA IES in the box*

$$\epsilon^L_{\mathrm{ssa}}(\mathbf{k}_L) := \inf_{\alpha,\theta}(\Psi_{\alpha,\theta,\mathbf{k}_L}|H^L\Psi_{\alpha,\theta,\mathbf{k}_L}) - E^L_{\mathrm{ssa}}$$

and for $\mathbf{k} \in \mathbb{R}^d$ we define the *SSA IES in the thermodynamic limit*

$$\epsilon_{\mathrm{ssa}}(\mathbf{k}) := \sup_{\delta>0}\left(\liminf_{L\to\infty}\left(\inf_{\mathbf{k}'_L\in\frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k}-\mathbf{k}'_L|<\delta}\epsilon^L_{\mathrm{ssa}}(\mathbf{k}'_L)\right)\right).$$

Clearly, from the mini-max principle we obtain:

$$E^L \le E^L_{\mathrm{ssa}}, \qquad E^L + \epsilon^L(\mathbf{k}_L) \le E^L_{\mathrm{ssa}} + \epsilon^L_{\mathrm{ssa}}(\mathbf{k}_L).$$

Conjecture 6.1. We believe the following statements to hold true:

(1) $\epsilon^L_{\mathrm{ssa}}(\mathbf{k}_L) > 0$ for all $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$.
(2) $\epsilon_{\mathrm{ssa}}(\mathbf{k}) > 0$, for all $\mathbf{k} \in \mathbb{R}^d$.
(3) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon_{\mathrm{ssa}}(\mathbf{k}) \in \mathbb{R}_+$ is continuous.
(4) Let $\mathbf{k} \in \mathbb{R}^d$. If $\{L_s\}_{s\ge1} \subset \mathbb{R}$ diverges to $+\infty$, then for every sequence $\mathbf{k}_s \in \frac{2\pi}{L_s}\mathbb{Z}^d$ which obeys $\mathbf{k}_s \to \mathbf{k}$, we have that $\epsilon^{L_s}_{\mathrm{ssa}}(\mathbf{k}_s) \to \epsilon_{\mathrm{ssa}}(\mathbf{k})$.

Thus we conjecture that the Squeezed States Approximation does not capture the behavior at the bottom of the IES predicted by Landau, in particular $\epsilon_{\mathrm{ssa}}(0) > 0$.

7. A rigorous version of the Bogoliubov approximation

The method of SSA is still not very convenient computationally. In this section we describe a less precise method of finding an upper bound to $E^L + \epsilon^L(\mathbf{k})$, which seems, however, more convenient in practical calculations. This method resembles closely the original Bogoliubov method. It consists of similar steps: it introduces a c-number α for the zero mode, it involves a "Bogoliubov rotation" and dropping terms of higher order in creation and annihilation operators. In contrast to the original Bogoliubov approach, our approach leads to a rigorous upper bound. Therefore, we call it the *Improved Bogoliubov Approximation* (IBA).

For any L large enough we assume that the infimum of $(\Psi_{\alpha,\theta}|H^L\Psi_{\alpha,\theta})$ is attained. Therefore, for any large enough L we can fix (α^L, θ^L), where $\alpha^L \in \mathbb{C}$ and $\frac{2\pi}{L}\mathbb{Z}^d \ni \mathbf{k} \mapsto \theta^L_{\mathbf{k}} \in \mathbb{C}$, such that

$$E^L_{\mathrm{ssa}} = (\Psi_{\alpha^L,\theta^L}|H^L\Psi_{\alpha^L,\theta^L}).$$

We define for $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$

$$\epsilon^L_{\mathrm{iba}}(\mathbf{k}_L) := (\Psi_{\alpha^L,\theta^L,\mathbf{k}_L}|H^L\Psi_{\alpha^L,\theta^L,\mathbf{k}_L}) - E^L_{\mathrm{ssa}}.$$

For $\mathbf{k} \in \mathbb{R}^d$ we set

$$\epsilon_{\mathrm{iba}}(\mathbf{k}) := \sup_{\delta>0}\left(\liminf_{L\to\infty}\left(\inf_{\mathbf{k}'_L\in\frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k}-\mathbf{k}'_L|<\delta}\epsilon^L_{\mathrm{iba}}(\mathbf{k}'_L)\right)\right).$$

Clearly,

$$\epsilon^L_{\mathrm{ssa}}(\mathbf{k}) \le \epsilon^L_{\mathrm{iba}}(\mathbf{k}), \qquad \epsilon_{\mathrm{ssa}}(\mathbf{k}) \le \epsilon_{\mathrm{iba}}(\mathbf{k}).$$

Again, we have a conjecture similar to the conjecture about the Squeezed States Approximation:

Conjecture 7.1. We believe the following statements to hold true:

(1) $\epsilon^L_{\mathrm{iba}}(\mathbf{k}_L) > 0$ for all $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$.
(2) $\epsilon_{\mathrm{iba}}(\mathbf{k}) > 0$ for all $\mathbf{k} \in \mathbb{R}^d$.
(3) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon_{\mathrm{iba}}(\mathbf{k}) \in \mathbb{R}_+$ is continuous.
(4) Let $\mathbf{k} \in \mathbb{R}^d$. If $\{L_s\}_{s\ge1} \subset \mathbb{R}$ diverges to $+\infty$, then for every sequence $\mathbf{k}_s \in \frac{2\pi}{L_s}\mathbb{Z}^d$ which obeys $\mathbf{k}_s \to \mathbf{k}$, we have that $\epsilon^{L_s}_{\mathrm{iba}}(\mathbf{k}_s) \to \epsilon_{\mathrm{iba}}(\mathbf{k})$.

In order to implement the above method, let us see that

$$(\Psi_{\alpha,\theta}|H^L\Psi_{\alpha,\theta}) = (\Omega|U_{\alpha,\theta}H^L U^*_{\alpha,\theta}\Omega),$$

$$(\Psi_{\alpha,\theta,\mathbf{k}_L}|H^L\Psi_{\alpha,\theta,\mathbf{k}_L}) = (a^*_{\mathbf{k}_L}\Omega|U_{\alpha,\theta}H^L U^*_{\alpha,\theta}a^*_{\mathbf{k}_L}\Omega).$$

The Hamiltonian after the Bogoliubov transformation can be Wick ordered:

$$\begin{aligned}U_{\alpha,\theta}H^L U^*_{\alpha,\theta} &= B^L + C^L a_0^* + \overline{C}^L a_0 \\ &+ \frac{1}{2}\sum_{\mathbf{k}} O^L(\mathbf{k})a^*_{\mathbf{k}}a^*_{-\mathbf{k}} + \frac{1}{2}\sum_{\mathbf{k}} \overline{O}^L(\mathbf{k})a_{\mathbf{k}}a_{-\mathbf{k}} + \sum_{\mathbf{k}} D^L(\mathbf{k})a^*_{\mathbf{k}}a_{\mathbf{k}} \\ &+ \text{terms higher order in } a\text{'s.}\end{aligned} \tag{7.1}$$

Then we easily see that

$$(\Psi_{\alpha,\theta}|H^L\Psi_{\alpha,\theta}) = B^L, \qquad (\Psi_{\alpha,\theta,\mathbf{k}}|H^L\Psi_{\alpha,\theta,\mathbf{k}}) = B^L + D^L(\mathbf{k}).$$

If we require that B^L attains its minimum, then we will later on show that automatically C^L and $O^L(\mathbf{k})$ vanish for all $\mathbf{k}$. Besides, we get that $B^L = E^L_{\mathrm{ssa}}$ and $D^L(\mathbf{k}) = \epsilon^L_{\mathrm{iba}}(\mathbf{k})$.

Note that it is natural to introduce the effective Hamiltonian

$$H^L_{\mathrm{iba}} := E^L_{\mathrm{ssa}} + \sum_{\mathbf{k}} \epsilon^L_{\mathrm{iba}}(\mathbf{k})b^*_{\mathbf{k}}b_{\mathbf{k}}, \tag{7.2}$$

where $b_{\mathbf{k}} = U_{\alpha,\theta}a_{\mathbf{k}}U^*_{\alpha,\theta}$. The elementary excitation spectrum of H^L_{iba} coincides with the IES of the full Hamiltonian H^L in the Improved Bogoliubov Approximation.

The method IBA seems especially convenient, not only as a means of obtaining an upper bound, but also as the first step to a systematic perturbative treatment of the Bose gas. We can use the effective Hamiltonian (7.2) as the main part of the full Hamiltonian H^L, treating the higher order terms dropped when defining (7.2) as a perturbation.

8. Bogoliubov translation of the Hamiltonian

In the sequel we drop the superscript L.

We apply the Bogoliubov transformation in two steps. First we apply $W_\alpha := \mathrm{e}^{-\alpha a_0^* + \overline{\alpha} a_0}$. We have $W_\alpha a_0 W^*_\alpha = a_0 + \alpha$. Hence it suffices to displace the zero mode and our Hamiltonian takes the form:

$$\begin{aligned}W_\alpha H W^*_\alpha &= -\mu|\alpha|^2 + \frac{\hat{v}(0)}{2V}|\alpha|^4 \\ &+ \left(\frac{\hat{v}(0)}{V}|\alpha|^2 - \mu\right)(\overline{\alpha}a_0 + \alpha a_0^*) \\ &+ \sum_{\mathbf{k}}\left(\frac{1}{2}\mathbf{k}^2 - \mu + \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}))}{V}|\alpha|^2\right)a^*_{\mathbf{k}}a_{\mathbf{k}} \\ &+ \sum_{\mathbf{k}}\frac{\hat{v}(\mathbf{k})}{2V}\left(\overline{\alpha}^2 a_{\mathbf{k}}a_{-\mathbf{k}} + a^*_{\mathbf{k}}a^*_{-\mathbf{k}}\alpha^2\right) \\ &+ \sum_{\mathbf{k},\mathbf{k}'}\frac{\hat{v}(\mathbf{k})}{V}(\overline{\alpha}a^*_{\mathbf{k}+\mathbf{k}'}a_{\mathbf{k}}a_{\mathbf{k}'} + \alpha a^*_{\mathbf{k}}a^*_{\mathbf{k}'}a_{\mathbf{k}+\mathbf{k}'}) \\ &+ \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\frac{\hat{v}(\mathbf{k}_2-\mathbf{k}_3)}{2V}a^*_{\mathbf{k}_1}a^*_{\mathbf{k}_2}a_{\mathbf{k}_3}a_{\mathbf{k}_4}.\end{aligned} \tag{8.1}$$

Before the displacement of the zero mode the Hamiltonian possessed global phase symmetry. After the displacement, the Hamiltonian will still have it if we also rotate the c-number α with the same phase as each operator $a_{\mathbf{k}}$.

9. Bogoliubov rotation of the Hamiltonian

Next we perform the Bogoliubov rotation by U_θ. We set

$$c_{\mathbf{k}} := \cosh|\theta_{\mathbf{k}}|, \quad s_{\mathbf{k}} := -\frac{\theta_{\mathbf{k}}}{|\theta_{\mathbf{k}}|}\sinh|\theta_{\mathbf{k}}|.$$

Note that

$$U_\theta a_{\mathbf{k}} U_\theta^* = c_{\mathbf{k}} a_{\mathbf{k}} - s_{\mathbf{k}} a_{-\mathbf{k}}^*, \quad U_\theta a_{\mathbf{k}}^* U_\theta^* = c_{\mathbf{k}} a_{\mathbf{k}}^* - \overline{s}_{\mathbf{k}} a_{-\mathbf{k}} \tag{9.1}$$

We have $s_{\mathbf{k}} = s_{-\mathbf{k}}$ and $c_{\mathbf{k}} = c_{-\mathbf{k}} = \sqrt{1+\overline{s}_{\mathbf{k}} s_{\mathbf{k}}}$.

The result of the rotation is:

$$\begin{aligned}
B &= -\mu|\alpha|^2 + \frac{\hat{v}(0)}{2V}|\alpha|^4 \\
&\quad + \sum_{\mathbf{k}} \left(\frac{\mathbf{k}^2}{2} - \mu + \frac{(\hat{v}(\mathbf{k}) + \hat{v}(0))}{V}|\alpha|^2\right)|s_{\mathbf{k}}|^2 \\
&\quad - \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{2V}(\overline{\alpha}^2 s_{\mathbf{k}} c_{\mathbf{k}} + \alpha^2 \overline{s}_{\mathbf{k}} c_{\mathbf{k}}) \\
&\quad + \sum_{\mathbf{k},\mathbf{k}'} \frac{\hat{v}(\mathbf{k}-\mathbf{k}')}{2V} c_{\mathbf{k}} s_{\mathbf{k}} c_{\mathbf{k}'} \overline{s}_{\mathbf{k}'} \\
&\quad + \sum_{\mathbf{k},\mathbf{k}'} \frac{\hat{v}(0) + \hat{v}(\mathbf{k}-\mathbf{k}')}{2V}|s_{\mathbf{k}}|^2|s_{\mathbf{k}'}|^2; \\
C &= \left(\frac{\hat{v}(0)}{V}|\alpha|^2 - \mu + \sum_{\mathbf{k}} \frac{(\hat{v}(0) + \hat{v}(\mathbf{k}))}{V}|s_{\mathbf{k}}|^2\right)(\alpha c_0 - \overline{\alpha} s_0) \\
&\quad + \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{V}\left(\alpha s_0 c_{\mathbf{k}} \overline{s}_{\mathbf{k}} - \overline{\alpha} c_0 c_{\mathbf{k}} s_{\mathbf{k}}\right);
\end{aligned}$$

$$\begin{aligned}
O(\mathbf{k}) &= -\left(\frac{\mathbf{k}^2}{2} - \mu + \frac{(\hat{v}(0) + \hat{v}(\mathbf{k}))}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{(\hat{v}(\mathbf{k}-\mathbf{k}') + \hat{v}(0))}{V}|s_{\mathbf{k}'}|^2\right) 2c_{\mathbf{k}} s_{\mathbf{k}} \\
&\quad + \left(\frac{\hat{v}(\mathbf{k})}{V}\alpha^2 - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{V} s_{\mathbf{k}'} c_{\mathbf{k}'}\right) c_{\mathbf{k}}^2 \\
&\quad + \left(\frac{\hat{v}(\mathbf{k})}{V}\overline{\alpha}^2 - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{V} \overline{s}_{\mathbf{k}'} c_{\mathbf{k}'}\right) s_{\mathbf{k}}^2; \\
D(\mathbf{k}) &= \left(\frac{\mathbf{k}^2}{2} - \mu + \frac{(\hat{v}(0) + \hat{v}(\mathbf{k}))}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(0) + \hat{v}(\mathbf{k}'-\mathbf{k})}{V}|s_{\mathbf{k}'}|^2\right)(c_{\mathbf{k}}^2 + |s_{\mathbf{k}}|^2) \\
&\quad - \left(\frac{\hat{v}(\mathbf{k})}{V}\alpha^2 - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{V} s_{\mathbf{k}'} c_{\mathbf{k}'}\right) c_{\mathbf{k}} \overline{s}_{\mathbf{k}} \\
&\quad - \left(\frac{\hat{v}(\mathbf{k})}{V}\overline{\alpha}^2 - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{V} \overline{s}_{\mathbf{k}'} c_{\mathbf{k}'}\right) s_{\mathbf{k}} c_{\mathbf{k}}.
\end{aligned}$$

The main intermediate step of the calculations leading to the above result is described in Appendix C.

10. Conditions arising from minimization of B

We demand that B attains a minimum. To this end we first compute the derivatives with respect to α and $\overline{\alpha}$: The first derivatives with respect to α and $\overline{\alpha}$ are:

$$
\begin{aligned}
\partial_\alpha B &= \left(-\mu + \frac{\hat{v}(0)}{V}|\alpha|^2 + \sum_{\mathbf{k}} \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}))}{V}|s_{\mathbf{k}}|^2\right)\overline{\alpha} \\
&\quad - \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{V}\overline{s}_{\mathbf{k}} c_{\mathbf{k}} \alpha, \\
\partial_{\overline{\alpha}} B &= \left(-\mu + \frac{\hat{v}(0)}{V}|\alpha|^2 + \sum_{\mathbf{k}} \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}))}{V}|s_{\mathbf{k}}|^2\right)\alpha \\
&\quad - \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{V} s_{\mathbf{k}} c_{\mathbf{k}} \overline{\alpha}.
\end{aligned}
$$

Note that

$$C = c_0 \partial_{\overline{\alpha}} B - s_0 \partial_\alpha B,$$

so that the condition

$$\partial_{\overline{\alpha}} B = \partial_\alpha B = 0 \tag{10.1}$$

entails $C = 0$.

Computing the derivative with respect to $s_{\mathbf{k}}$, $\overline{s}_{\mathbf{k}}$ we can use

$$\partial_{s_{\mathbf{k}}} c_{\mathbf{k}} = \frac{\overline{s}_{\mathbf{k}}}{2c_{\mathbf{k}}}, \quad \partial_{\overline{s}_{\mathbf{k}}} c_{\mathbf{k}} = \frac{s_{\mathbf{k}}}{2c_{\mathbf{k}}}.$$

$$
\begin{aligned}
\partial_{s_{\mathbf{k}}} B &= \left(\frac{\mathbf{k}^2}{2} - \mu + \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}))}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}'-\mathbf{k}))}{V}|s_{\mathbf{k}'}|^2\right)\overline{s}_{\mathbf{k}} \\
&\quad + \left(-\frac{\hat{v}(\mathbf{k})}{2V}\overline{\alpha}^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{2V} c_{\mathbf{k}'}\overline{s}_{\mathbf{k}'}\right)\left(c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{2c_{\mathbf{k}}}\right) \\
&\quad + \left(-\frac{\hat{v}(\mathbf{k})}{2V}\alpha^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{2V} c_{\mathbf{k}'} s_{\mathbf{k}'}\right)\frac{\overline{s}_{\mathbf{k}}^2}{2c_{\mathbf{k}}}; \\
\partial_{\overline{s}_{\mathbf{k}}} B &= \left(\frac{\mathbf{k}^2}{2} - \mu + \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}))}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{(\hat{v}(0)+\hat{v}(\mathbf{k}'-\mathbf{k}))}{V}|s_{\mathbf{k}'}|^2\right) s_{\mathbf{k}} \\
&\quad + \left(-\frac{\hat{v}(\mathbf{k})}{2V}\alpha^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{2V} c_{\mathbf{k}'} s_{\mathbf{k}'}\right)\left(c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{2c_{\mathbf{k}}}\right) \\
&\quad + \left(-\frac{\hat{v}(\mathbf{k})}{2V}\overline{\alpha}^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{2V} c_{\mathbf{k}'}\overline{s}_{\mathbf{k}'}\right)\frac{s_{\mathbf{k}}^2}{2c_{\mathbf{k}}}.
\end{aligned}
$$

One can calculate that

$$O(\mathbf{k}) = \left(-2c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{c_{\mathbf{k}}}\right)\partial_{\overline{s}_{\mathbf{k}}} B - \frac{s_{\mathbf{k}}^2}{c_{\mathbf{k}}}\partial_{s_{\mathbf{k}}} B.$$

Thus $\partial_{s_{\mathbf{k}}} B = \partial_{\overline{s}_{\mathbf{k}}} B = 0$ entails $O(\mathbf{k}) = 0$.

All the above conditions can be rewritten using

$$
\begin{aligned}
f_{\mathbf{k}}: &= \frac{\mathbf{k}^2}{2} - \mu \\
&\quad + |\alpha|^2 \frac{\hat{v}(0) + \hat{v}(\mathbf{k})}{V} + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}' - \mathbf{k}) + \hat{v}(0)}{V} |s_{\mathbf{k}'}|^2, \\
g_{\mathbf{k}}: &= \alpha^2 \frac{\hat{v}(\mathbf{k})}{V} - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}' - \mathbf{k})}{V} s_{\mathbf{k}'} c_{\mathbf{k}'}.
\end{aligned} \tag{10.2}
$$

Note that $f_{\mathbf{k}}$ is real. Then:

$$
\begin{aligned}
\partial_{s_{\mathbf{k}}} B &= f_{\mathbf{k}} \overline{s}_{\mathbf{k}} - \frac{\overline{g}_{\mathbf{k}}}{2} \left(c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{2c_{\mathbf{k}}} \right) - g_{\mathbf{k}} \frac{\overline{s}_{\mathbf{k}}^2}{4c_{\mathbf{k}}}, \\
\partial_{\overline{s}_{\mathbf{k}}} B &= f_{\mathbf{k}} s_{\mathbf{k}} - \frac{g_{\mathbf{k}}}{2} \left(c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{2c_{\mathbf{k}}} \right) - \overline{g}_{\mathbf{k}} \frac{s_{\mathbf{k}}^2}{4c_{\mathbf{k}}}.
\end{aligned}
$$

and

$$
s_{\mathbf{k}} \partial_{s_{\mathbf{k}}} B - \overline{s}_{\mathbf{k}} \partial_{\overline{s}_{\mathbf{k}}} B = \frac{c_{\mathbf{k}}}{2} (g_{\mathbf{k}} \overline{s}_{\mathbf{k}} - \overline{g}_{\mathbf{k}} s_{\mathbf{k}}).
$$

This implies that

$$
g_{\mathbf{k}} \overline{s}_{\mathbf{k}} = \overline{g}_{\mathbf{k}} s_{\mathbf{k}}. \tag{10.3}
$$

Note also that we can use $f_{\mathbf{k}}$ and $g_{\mathbf{k}}$ to write (without minimizing)

$$
D(\mathbf{k}) = f_{\mathbf{k}} (c_{\mathbf{k}}^2 + |s_{\mathbf{k}}|^2) - c_{\mathbf{k}} (s_{\mathbf{k}} \overline{g}_{\mathbf{k}} + \overline{s}_{\mathbf{k}} g_{\mathbf{k}}), \tag{10.4}
$$

$$
O(\mathbf{k}) = -2 c_{\mathbf{k}} s_{\mathbf{k}} f_{\mathbf{k}} + s_{\mathbf{k}}^2 \overline{g}_{\mathbf{k}} + c_{\mathbf{k}}^2 g_{\mathbf{k}}. \tag{10.5}
$$

The condition (10.1) yields

$$
\mu = \frac{\hat{v}(0)}{V} |\alpha|^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(0) + \hat{v}(\mathbf{k}')}{V} |s_{\mathbf{k}'}|^2 - \frac{\alpha^2}{|\alpha|^2} \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{V} \overline{s}_{\mathbf{k}'} c_{\mathbf{k}'}. \tag{10.6}
$$

This allows to eliminate μ from the expression for $f_{\mathbf{k}}$:

$$
\begin{aligned}
f_{\mathbf{k}}: &= \frac{\mathbf{k}^2}{2} + |\alpha|^2 \frac{\hat{v}(\mathbf{k})}{V} \\
&\quad + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}' - \mathbf{k}) - \hat{v}(\mathbf{k}')}{V} |s_{\mathbf{k}'}|^2 + \frac{\alpha^2}{|\alpha|^2} \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{V} \overline{s}_{\mathbf{k}'} c_{\mathbf{k}'}.
\end{aligned} \tag{10.7}
$$

We will keep α^2 instead of μ as the parameter of the theory, hoping that one can later on express μ in terms of α^2.

One can express the minimizing conditions in the following theorem.

Theorem 10.1. *Suppose that $\mu > 0$. Let the first derivative of B with respect to $\alpha, \overline{\alpha}, (s_{\mathbf{k}}), (\overline{s}_{\mathbf{k}})$ vanish. Let $f_{\mathbf{k}}$ and $g_{\mathbf{k}}$ be given by (10.7) and (10.2) and let μ be expressed by (10.6). Let $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$.*

(1) $f_{\mathbf{k}}^2 \geq |g_{\mathbf{k}}|^2$.
(2) $D(\mathbf{k}) = 0$ iff $f_{\mathbf{k}} = 0$.
(3) $D(\mathbf{k}) \neq 0$ iff $f_{\mathbf{k}}^2 > |g_{\mathbf{k}}|^2$. Then $s_{\mathbf{k}}$ solves the equation

$$
\begin{aligned}
s_{\mathbf{k}} &= \mathrm{sign} f_{\mathbf{k}} \frac{g_{\mathbf{k}}}{|g_{\mathbf{k}}|} \left(\frac{|f_{\mathbf{k}}| - \sqrt{f_{\mathbf{k}}^2 - |g_{\mathbf{k}}|^2}}{2\sqrt{f_{\mathbf{k}}^2 - |g_{\mathbf{k}}|^2}} \right)^{1/2}, \quad && g_{\mathbf{k}} \neq 0 \\
s_{\mathbf{k}} &= 0, && g_{\mathbf{k}} = 0.
\end{aligned} \tag{10.8}
$$

We have then

$$
D(\mathbf{k}) = \mathrm{sign} f_{\mathbf{k}} \sqrt{f_{\mathbf{k}}^2 - |g_{\mathbf{k}}|^2}. \tag{10.9}
$$

(4) We have

$$\begin{bmatrix} \partial_{\overline{\alpha}}\partial_\alpha B & \partial_{\overline{\alpha}}^2 B \\ \partial_\alpha^2 B & \partial_\alpha\partial_{\overline{\alpha}} B \end{bmatrix} = \begin{bmatrix} f_0 & g_0 \\ \overline{g}_0 & f_0 \end{bmatrix}. \tag{10.10}$$

(10.10) is positive/negative definite iff $D(0)$ is positive/negative. Besides,

$$D(0) = 2\mathrm{sign} f_0 \sqrt{\frac{\hat{v}(0)}{V}\alpha^2 \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{V}\overline{s}_{\mathbf{k}} c_{\mathbf{k}}}$$

Proof. We can use (10.3) to rewrite (10.4) and (10.5) as

$$\begin{aligned} D(\mathbf{k}) &= f_{\mathbf{k}}(c_{\mathbf{k}}^2 + |s_{\mathbf{k}}|^2) - 2c_{\mathbf{k}} s_{\mathbf{k}} \overline{g}_{\mathbf{k}}, \\ O(\mathbf{k}) &= -2c_{\mathbf{k}} s_{\mathbf{k}} f_{\mathbf{k}} + (|s_{\mathbf{k}}|^2 + c_{\mathbf{k}}^2) g_{\mathbf{k}}. \end{aligned}$$

The condition $O(\mathbf{k}) = 0$ implies

$$2\sqrt{1+|s_{\mathbf{k}}|^2} s_{\mathbf{k}} f_{\mathbf{k}} = (1 + 2|s_{\mathbf{k}}|^2) g_{\mathbf{k}}. \tag{10.11}$$

Hence

$$4(|s_{\mathbf{k}}|^4 + |s_{\mathbf{k}}|^2)(f_{\mathbf{k}}^2 - |g_{\mathbf{k}}|^2) = |g_{\mathbf{k}}|^2. \tag{10.12}$$

Therefore $f_{\mathbf{k}}^2 \geq |g_{\mathbf{k}}|^2$.

If $f_{\mathbf{k}} = 0$, then $g_{\mathbf{k}} = 0$, and hence $D(\mathbf{k}) = 0$.

By (10.12), $f_{\mathbf{k}}^2 = |g_{\mathbf{k}}|^2$ implies $g_{\mathbf{k}} = 0$. Hence $f_{\mathbf{k}} = 0$ and $D(\mathbf{k}) = 0$.

If $f_{\mathbf{k}}^2 > |g_{\mathbf{k}}|^2$, then we easily derive (10.9), which shows that $D(\mathbf{k}) \neq 0$ and the sign of $f_{\mathbf{k}}$ and $D(\mathbf{k})$ coincide. □

Note that if we have $D(\mathbf{k}) < 0$ for some $\mathbf{k}$, then our method gives no useful results. This is equivalent to $f_{\mathbf{k}} < 0$. Therefore, physically the only interesting case of the above theorem corresponds to $f_{\mathbf{k}} \geq 0$.

The positivity of (10.10) is a necessary condition for the existence of minimum of B. Note that it implies that $D(0) > 0$.

Theorem 10.1 suggests the following iterative procedure for finding $\alpha, (s_{\mathbf{k}})$ satisfying the minimization condition. We start form $s_{\mathbf{k}} = 0$. Then, by (10.6),

$$\mu = \frac{\hat{v}(0)}{V}|\alpha|^2.$$

Inserting α and $s_{\mathbf{k}} = 0$ in (10.7) and (10.2) gives

$$f_{\mathbf{k}} = \frac{\mathbf{k}^2}{2} + |\alpha|^2 \frac{\hat{v}(\mathbf{k})}{V}, \tag{10.13}$$

$$g_{\mathbf{k}} = \alpha^2 \frac{\hat{v}(\mathbf{k})}{V}. \tag{10.14}$$

Note that $\hat{v}(\mathbf{k}) \geq 0$ implies that $f_{\mathbf{k}} \geq 0$. Inserting (10.13) and (10.14) into (10.8) we obtain

$$\begin{aligned} s_{\mathbf{k}} &= \frac{\alpha}{\sqrt{2}|\alpha|}\left(\left(1 - \left(\frac{\hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(0)}}{\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(0)}}\right)^2\right)^{-1/2} - 1\right)^{1/2}. \\ D(\mathbf{k}) &= \sqrt{\frac{\mathbf{k}^2}{2}\left(\frac{\mathbf{k}^2}{2} + 2\hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(0)}\right)}, \end{aligned}$$

which coincide with the formulas for $s_{\mathbf{k}}$ and $\omega_{\mathrm{bg},\mu}(\mathbf{k})$ obtained in the grand-canonical version of the original Bogoliubov approximation (replace ρ in (2.10) and (2.6) with $\frac{\mu}{\hat{v}(0)}$).

Let us compute the ground state energy in the Squeezed States Approximation. Inserting (10.6) to the expression for B we obtain

$$\begin{aligned} B &= -\frac{\hat{v}(0)}{2V}\left(|\alpha|^2+\sum_{\mathbf{k}}|s_{\mathbf{k}}|^2\right)^2+\sum_{\mathbf{k}}\frac{\mathbf{k}^2}{2}|s_{\mathbf{k}}|^2 \\ &\quad +\sum_{\mathbf{k}}\frac{\hat{v}(\mathbf{k}-\mathbf{k}')-\hat{v}(\mathbf{k}')-v(\mathbf{k})}{2V}|s_{\mathbf{k}'}|^2|s_{\mathbf{k}}|^2 \\ &\quad +\sum_{\mathbf{k}}\frac{\hat{v}(\mathbf{k}')}{V}\frac{\alpha^2}{|\alpha|^2}\overline{s}_{\mathbf{k}'}c_{\mathbf{k}'}|s_{\mathbf{k}}|^2 \\ &\quad +\sum_{\mathbf{k}}\frac{\hat{v}(\mathbf{k}-\mathbf{k}')}{2V}c_{\mathbf{k}'}s_{\mathbf{k}'}c_{\mathbf{k}}\overline{s}_{\mathbf{k}}. \end{aligned}$$

Using (10.6) again to eliminate $|\alpha|^2$ in favor of μ, and then computing the derivative with respect to μ we obtain

$$-\partial_\mu B=|\alpha|^2+\sum_{\mathbf{k}}|s_{\mathbf{k}}|^2.$$

Therefore, the grand-canonical density is given by

$$\rho=\frac{|\alpha|^2+\sum_{\mathbf{k}}|s_{\mathbf{k}}|^2}{V}. \tag{10.15}$$

Note that it seems that in the thermodynamic limit one should take $\alpha=\sqrt{V\rho_0}\,\mathrm{e}^{\mathrm{i}\phi_0}$, for some fixed parameter ρ_0 having the interpretation of the density of the condensate and a fixed phase ϕ_0. Then one could expect that $s_{\mathbf{k}}$ will converge to a function depending on $\mathbf{k}\in\mathbb{R}^d$ in a reasonable class and we can replace $\frac{1}{V}\sum\limits_{\mathbf{k}}$ by $\frac{1}{(2\pi)^d}\int\mathrm{d}\mathbf{k}$. In particular, we obtain (in the physical case of positive D)

$$D(0)=2\sqrt{\hat{v}(0)\rho_0\frac{1}{(2\pi)^d}\int\mathrm{d}\mathbf{k}\hat{v}(\mathbf{k})\overline{s}_{\mathbf{k}}c_{\mathbf{k}}}.$$

Appendix A. Energy-momentum spectrum of quadratic Hamiltonians

Suppose that we consider a quantum system described by the Hamiltonian

$$H=\int_{\mathbb{R}^d}\omega(\mathbf{k})a_{\mathbf{k}}^*a_{\mathbf{k}}\mathrm{d}\mathbf{k}, \tag{A.1}$$

with the the total momentum

$$P=\int_{\mathbb{R}^d}\mathbf{k}a_{\mathbf{k}}^*a_{\mathbf{k}}\mathrm{d}\mathbf{k},$$

both acting on the Fock space $\Gamma_{\mathrm{s}}(L^2(\mathbb{R}^d))$. We will call the function ω appearing in H the *elementary excitation spectrum* of our quantum system and we will assume it to be nonnegative.

Clearly, the ground state energy of H is 0. In this appendix we will discuss a possible shape of the energy-momentum spectrum, which in this case coincides with the excitation spectrum. First note that the excitation spectrum of (A.1) is not arbitrary. We will show that there is a large class of quadratic Hamiltonians for which the excitation spectrum has the properties described by Conjecture 4.3 (3) or (3)', and (4).

The results of this appendix strictly speaking do not apply to the Hamiltonian of Bose gas, since it is not purely quadratic. Nevertheless, it applies to its Bogoliubov approximation, which is quadratic, and which is believed to capture some features of the full Hamiltonian in the thermodynamic limit. They are very simple and probably they mostly belong to the folk wisdom. However, we have never seen them explicitly described in the literature.

Let $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon(\mathbf{k}) \in \mathbb{R}$ be a nonnegative function. We say that it is *subadditive* iff

$$\epsilon(\mathbf{k}_1 + \mathbf{k}_2) \leq \epsilon(\mathbf{k}_1) + \epsilon(\mathbf{k}_2), \quad \mathbf{k}_1, \mathbf{k}_2 \in \mathbb{R}^d.$$

Let $\mathbb{R}^d \ni \mathbf{k} \mapsto \omega(\mathbf{k}) \in \mathbb{R}$ be another nonnegative function. We define the *subbadditive envelope of* ω to be

$$\epsilon(\mathbf{k}) := \inf\{\omega(\mathbf{k}_1) + \cdots + \omega(\mathbf{k}_n) \ : \ \mathbf{k}_1 + \cdots + \mathbf{k}_n = \mathbf{k}, \ n = 1, 2, \dots\}.$$

Clearly, $\epsilon(\mathbf{k})$ is subadditive and satisfies $\epsilon(\mathbf{k}) \leq \omega(\mathbf{k})$.

Clearly, if $\omega(\mathbf{k})$ is the elementary excitation spectrum of a quadratic Hamiltonian, and ϵ its subadditive envelope, then $\epsilon(\mathbf{k})$ is the infimum of its excitation spectrum.

Let us state and prove some facts about subadditive functions and subadditive envelopes, which seem to be relevant for the homogeneous Bose gas.

Theorem A.1. *Let f be an increasing concave function on $[0, \infty[$ with $f(0) \geq 0$. Then $f(|\mathbf{k}|)$ is subadditive.*

Proof.

$$\begin{aligned}
f(|\mathbf{k}_1 + \mathbf{k}_2|) &\leq f(|\mathbf{k}_1| + |\mathbf{k}_2|) \\
&\leq \frac{|\mathbf{k}_1|}{|\mathbf{k}_1| + |\mathbf{k}_2|} f(|\mathbf{k}_1| + |\mathbf{k}_2|) + \frac{|\mathbf{k}_2|}{|\mathbf{k}_1| + |\mathbf{k}_2|} f(0) \\
&\quad + \frac{|\mathbf{k}_2|}{|\mathbf{k}_1| + |\mathbf{k}_2|} f(|\mathbf{k}_1| + |\mathbf{k}_2|) + \frac{|\mathbf{k}_1|}{|\mathbf{k}_1| + |\mathbf{k}_2|} f(0) \\
&\leq f(|\mathbf{k}_1|) + f(|\mathbf{k}_2|).
\end{aligned}$$

□

We can generalize Theorem A.1 to periodic functions.

Theorem A.2. *Let f be an increasing concave function on $[0, \frac{\sqrt{d}}{2}]$ with $f(0) \geq 0$. Define ϵ to be the function on $\mathbb{R}^d$ periodic with respect to the lattice $\mathbb{Z}^d$ such that if $\mathbf{k} \in [-\frac{1}{2}, \frac{1}{2}]^d$, then $\epsilon(\mathbf{k}) = f(|\mathbf{k}|)$ (which defines ϵ uniquely). Then ϵ is subadditive.*

Proof. We can extend f to a concave increasing function defined on $[0, \infty[$, e.g. by putting $f(t) = f(\frac{\sqrt{d}}{2})$ for $t \geq \frac{\sqrt{d}}{2}$.

Let $\mathbf{k}_1, \mathbf{k}_2 \in \mathbb{R}^d$. Let $\mathbf{p}_1, \mathbf{p}_2 \in [-\frac{1}{2}, \frac{1}{2}]^d$ such that $\mathbf{k}_i - \mathbf{p}_i \in \mathbb{Z}^d$. Let $\mathbf{p} \in [-\frac{1}{2}, \frac{1}{2}]^d$ such that $\mathbf{k}_i + \mathbf{k}_2 - \mathbf{p} \in \mathbb{Z}^d$. Note that $|\mathbf{p}| \leq |\mathbf{p}_1 + \mathbf{p}_2|$. Now

$$\begin{aligned}
\epsilon(\mathbf{k}_1 + \mathbf{k}_2) &= f(|\mathbf{p}|) \leq f(|\mathbf{p}_1 + \mathbf{p}_2|) \\
&\leq \cdots \\
&\leq f(|\mathbf{p}_1|) + f(|\mathbf{p}_2|) = \epsilon(\mathbf{k}_1) + \epsilon(\mathbf{k}_2),
\end{aligned}$$

where in ... we repeat the estimate of the proof of Theorem A.1. □

Obviously, we have

Theorem A.3. *Let ϵ_0 be subadditive and $\epsilon_0 \leq \omega$. Let ϵ be the subadditive envelope of ω. Then $\epsilon_0 \leq \epsilon$.*

In the case of the Bose gas with repulsive interactions we expect that the excitation spectrum may have resemble that of a quadratic Hamiltonian with the properties described by the following theorem, which easily follows from Theorems A.1, A.2 and A.3:

Theorem A.4. *Suppose that $\omega \geq 0$ and ϵ is its subadditive envelope.*

(1) If $\inf_{\mathbf{k} \neq 0} \frac{\omega(\mathbf{k})}{|\mathbf{k}|} = c$, then $\inf_{\mathbf{k} \neq 0} \frac{\epsilon(\mathbf{k})}{|\mathbf{k}|} = c$.

(2) If $\liminf_{\mathbf{k}\to 0}\frac{\omega(\mathbf{k})}{|\mathbf{k}|}=c$*, then* $\epsilon(\mathbf{k})\leq c|\mathbf{k}|$.

(3) Suppose that for some $c>0$*, we have* $\omega(\mathbf{k})\geq c\min(|\mathbf{k}|,1)$*. Then*

$$\liminf_{\mathbf{k}\to 0}\frac{\omega(\mathbf{k})}{|\mathbf{k}|}=c_{\mathrm{s}}\quad\textit{implies}\quad\lim_{\mathbf{k}\to 0}\frac{\epsilon(\mathbf{k})}{|\mathbf{k}|}=c_{\mathrm{s}}.$$

(4) If $\omega(\mathbf{k})$ *is periodic with respect to* $\mathbb{Z}^d$*, then so is* $\epsilon(\mathbf{k})$*.*

(5) Let $\omega(\mathbf{k})$ *be periodic with respect to* $\mathbb{Z}^d$*, and, for some* $c>0$*, we have* $\omega(\mathbf{k})\geq c\min\big(\mathrm{dist}(\mathbf{k},\mathbb{Z}^d),1\big)$*. Then*

$$\liminf_{\mathbf{k}\to 0}\frac{\omega(\mathbf{k})}{|\mathbf{k}|}=c_{\mathrm{s}}\quad\textit{implies}\quad\lim_{\mathbf{k}\to 0}\frac{\epsilon(\mathbf{k})}{|\mathbf{k}|}=c_{\mathrm{s}}.$$

Appendix B. Bogoliubov transformations

In this appendix we recall the well-known properties of Bogoliubov transformations and squeezed vectors. For simplicity we restrict ourselves to one degree of freedom.

Let a^*, a are creation and annihilation operators and Ω the vacuum vector. Recall that $[a,a^*]=1$ and $a\Omega=0$.

Here are the basic identities for Bogoliubov translations and coherent vectors. Let

$$W:=\mathrm{e}^{-\alpha a^*+\overline{\alpha}a}.$$

Then

$$\begin{aligned} WaW^* &= a+\alpha,\\ Wa^*W^* &= a^*+\overline{\alpha},\\ W^*\Omega &= \mathrm{e}^{-\frac{|\alpha|^2}{2}}\,\mathrm{e}^{\alpha a^*}\,\Omega. \end{aligned}$$

Here are the basic identities for Bogoliubov rotations and squeezed vectors. Let

$$U:=\mathrm{e}^{-\frac{\theta}{2}a^*a^*+\frac{\overline{\theta}}{2}aa}.$$

Then

$$\begin{aligned} UaU^* &= \cosh|\theta|a+\tfrac{\theta}{|\theta|}\sinh|\theta|a^*,\\ Ua^*U^* &= \cosh|\theta|a^*+\tfrac{\overline{\theta}}{|\theta|}\sinh|\theta|a,\\ U^*\Omega &= (1+\tanh^2|\theta|)^{\frac14}\,\mathrm{e}^{-\frac{\theta}{2|\theta|}\tanh|\theta|a^*a^*}\,\Omega. \end{aligned}$$

Vectors obtained by acting with both Bogoliubov translation and rotation will be also called squeezed vectors.

Appendix C. Computations of the Bogoliubov rotation

In this appendix we give the computations of the rotated terms in the Hamiltonian used in Section 9.

$$\begin{aligned} U_\theta a^*_{\mathbf{k}}a_{\mathbf{k}}U^*_\theta &= |s_{\mathbf{k}}|^2\\ &\quad +c^2_{\mathbf{k}}a^*_{\mathbf{k}}a_{\mathbf{k}}-c_{\mathbf{k}}s_{\mathbf{k}}a^*_{\mathbf{k}}a^*_{-\mathbf{k}}-c_{\mathbf{k}}\overline{s}_{\mathbf{k}}a_{\mathbf{k}}a_{-\mathbf{k}}+|s_{\mathbf{k}}|^2a^*_{-\mathbf{k}}a_{-\mathbf{k}},\\ U_\theta a^*_{\mathbf{k}}a^*_{-\mathbf{k}}U^*_\theta &= -\overline{s}_{\mathbf{k}}c_{\mathbf{k}}\\ &\quad +c^2_{\mathbf{k}}a^*_{\mathbf{k}}a^*_{-\mathbf{k}}-c_{\mathbf{k}}\overline{s}_{\mathbf{k}}a^*_{\mathbf{k}}a_{\mathbf{k}}-c_{\mathbf{k}}\overline{s}_{\mathbf{k}}a^*_{-\mathbf{k}}a_{-\mathbf{k}}+\overline{s}^2_{\mathbf{k}}a_{-\mathbf{k}}a_{\mathbf{k}};\\ U_\theta a_{\mathbf{k}}a_{-\mathbf{k}}U^*_\theta &= -s_{\mathbf{k}}c_{\mathbf{k}}\\ &\quad +c^2_{\mathbf{k}}a_{\mathbf{k}}a_{-\mathbf{k}}-c_{\mathbf{k}}s_{\mathbf{k}}a^*_{\mathbf{k}}a_{\mathbf{k}}-c_{\mathbf{k}}s_{\mathbf{k}}a^*_{-\mathbf{k}}a_{-\mathbf{k}}+s^2_{\mathbf{k}}a^*_{-\mathbf{k}}a^*_{\mathbf{k}}; \end{aligned}$$

$$
\begin{aligned}
U_\theta a^*_{\mathbf{k}+\mathbf{k}'} a_{\mathbf{k}} a_{\mathbf{k}'} U^*_\theta &= \big(c_0(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + \overline{s}_0 c_{\mathbf{k}} s_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a_0 \\
&\quad - \big(s_0(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + c_0 \overline{c}_{\mathbf{k}} s_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a^*_0 \\
&\quad + \text{higher order terms;} \\
U_\theta a_{\mathbf{k}+\mathbf{k}'} a^*_{\mathbf{k}} a^*_{\mathbf{k}'} U^*_\theta &= \big(c_0(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + s_0 c_{\mathbf{k}} \overline{s}_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a^*_0 \\
&\quad - \big(\overline{s}_0(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + c_0 c_{\mathbf{k}} \overline{s}_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a_0 \\
&\quad + \text{higher order terms;}
\end{aligned}
$$

$$
\begin{aligned}
& \delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4) U_\theta a^*_{\mathbf{k}_1} a^*_{\mathbf{k}_2} a_{\mathbf{k}_3} a_{\mathbf{k}_4} U^*_\theta \\
= \;& c_{\mathbf{k}_1} \overline{s}_{\mathbf{k}_1} c_{\mathbf{k}_3} s_{\mathbf{k}_3} \delta(\mathbf{k}_1+\mathbf{k}_2)\delta(\mathbf{k}_3+\mathbf{k}_4) \\
+ \;& |s_{\mathbf{k}_1}|^2 |s_{\mathbf{k}_2}|^2 \left(\delta(\mathbf{k}_1-\mathbf{k}_3)\delta(\mathbf{k}_2-\mathbf{k}_4) + \delta(\mathbf{k}_1-\mathbf{k}_4)\delta(\mathbf{k}_2-\mathbf{k}_3)\right) \\
+ \;& \Big(\overline{s}_{\mathbf{k}_1} c_{\mathbf{k}_1} (s_{\mathbf{k}_3} c_{\mathbf{k}_3} a^*_{-\mathbf{k}_3} a_{-\mathbf{k}_3} - s^2_{\mathbf{k}_3} a^*_{\mathbf{k}_3} a^*_{-\mathbf{k}_3} - c^2_{\mathbf{k}_3} a_{\mathbf{k}_3} a_{-\mathbf{k}_3} + s_{\mathbf{k}_3} c_{\mathbf{k}_3} a^*_{\mathbf{k}_3} a_{\mathbf{k}_3}) \\
& + s_{\mathbf{k}_3} c_{\mathbf{k}_3} (\overline{s}_{\mathbf{k}_1} c_{\mathbf{k}_1} a^*_{\mathbf{k}_1} a_{\mathbf{k}_1} - \overline{s}^2_{\mathbf{k}_1} a_{\mathbf{k}_1} a_{-\mathbf{k}_1} - c^2_{\mathbf{k}_1} a^*_{\mathbf{k}_1} a^*_{-\mathbf{k}_1} + \overline{s}_{\mathbf{k}_1} c_{\mathbf{k}_1} a^*_{-\mathbf{k}_1} a_{-\mathbf{k}_1})\Big) \\
& \times \delta(\mathbf{k}_1+\mathbf{k}_2)\delta(\mathbf{k}_3+\mathbf{k}_4) \\
+ \;& \Big(|s_{\mathbf{k}_2}|^2 (|c_{\mathbf{k}_1}|^2 a^*_{\mathbf{k}_1} a_{\mathbf{k}_1} - c_{\mathbf{k}_1} s_{\mathbf{k}_1} a^*_{\mathbf{k}_1} a^*_{-\mathbf{k}_1} - c_{\mathbf{k}_1} \overline{s}_{\mathbf{k}_1} a_{\mathbf{k}_1} a_{-\mathbf{k}_1} + |s_{\mathbf{k}_1}|^2 a^*_{-\mathbf{k}_1} a_{-\mathbf{k}_1}) \\
& + |s_{\mathbf{k}_1}|^2 (|c_{\mathbf{k}_2}|^2 a^*_{\mathbf{k}_2} a_{\mathbf{k}_2} - c_{\mathbf{k}_2} s_{\mathbf{k}_2} a^*_{\mathbf{k}_2} a^*_{-\mathbf{k}_2} - c_{\mathbf{k}_2} \overline{s}_{\mathbf{k}_2} a_{\mathbf{k}_2} a_{-\mathbf{k}_2} + |s_{\mathbf{k}_2}|^2 a^*_{-\mathbf{k}_2} a_{-\mathbf{k}_2})\big) \\
& \times \big(\delta(\mathbf{k}_1-\mathbf{k}_3)\delta(\mathbf{k}_2-\mathbf{k}_4) + \delta(\mathbf{k}_1-\mathbf{k}_4)\delta(\mathbf{k}_2-\mathbf{k}_3)\Big) \\
& + \text{higher order terms.}
\end{aligned}
$$

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(H.D. Cornean) Dept. of Math., Aalborg University, Fredrik Bajers Vej 7G, 9220 Aalborg, Denmark
E-mail address: cornean@math.aau.dk

(J. Dereziński) Dept. of Math. Methods in Phys., University of Warsaw, Hoza 74, 00-682 Warszawa, Poland
E-mail address: Jan.Derezinski@fuw.edu.pl

(P. Ziń) Institute of Theoretical Physics, Uniwersity of Warsaw, Hoza 69, 00-681 Warszawa, Poland
E-mail address: Pawel.Zin@fuw.edu.pl