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

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Abstract. We consider second quantized homogeneous Bose gas in a large cubic box with periodic boundary conditions, at zero temperature. We discuss the energy-momentum spectrum of the Bose gas and its physical significance. We review various rigorous and heuristic results as well as open conjectures about its properties. Our main aim is to convince the readers, including those with mainly mathematical background, that this subject has many interesting problems for rigorous research.

In particular, we investigate the upper bound on the infimum of the energy for a fixed total momentum $\mathbf{k}$ given by the expectation value of one-particle excitations over a squeezed states. This bound can be viewed as a rigorous version of the famous Bogoliubov method. We show that this approach seems to lead to a (non-physical) energy gap.

The variational problem involving squeezed states can serve as the preparatory step in a perturbative approach that should be useful in computing excitation spectrum. This version of a perturbative approach to the Bose gas seems (at least in principle) superior to the commonly used approach based on the c-number substitution.

Contents

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1. Introduction

In this paper we would like to review one of outstanding open problems of quantum physics – rigorous understanding of the energy–momentum spectrum of homogeneous Bose gas at zero temperature. We describe various rigorous and heuristic arguments about its shape. In particular, we discuss a number of versions of the so-called Bogoliubov approach. We use the main idea of this approach to give rigorous upper bounds on the energy-momentum spectrum of the Bose gas.

There exists little rigorous work on this subject. We think that mathematicians avoid this topic not only because of its difficulty. Unfortunately, it is not easy to formulate questions in this domain that are, on one hand, physically relevant, and on the other hand, mathematically clean and precise. We try to ask a number of such questions, some of them rather ambitious, but some, perhaps, within the reach of present methods. We think that rigorous methods of spectral analysis and operator theory could be very helpful in clarifying this subject.

1.1. **Bose gas in canonical approach.** One can distinguish two possible approaches to the Bose gas at positive density: "canonical" – fixing the density ρ – and "grand-canonical" – fixing the chemical potential μ. In most of our paper we will concentrate on the latter setting. Nevertheless, in the introduction, as well as in Section 2, we will stick to the canonical approach.

We 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 $v(\mathbf{x})$ 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

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

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

Homogeneous Bose gas is described by the Hilbert space $L^2_{\mathrm{s}}((\mathbb{R}^d)^n)$ (symmetric square integrable functions on $(\mathbb{R}^d)^n$), the n-body Schrödinger Hamiltonian

$$H^n = -\sum_{i=1} \frac{1}{2}\Delta_i + \sum_{1\leq i<j\leq n} v(\mathbf{x}_i - \mathbf{x}_j) \tag{1.3}$$

and the momentum operator

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

(H, P) is a collection of $1 + d$ commuting self-adjoint operators, hence we can ask about the properties of their joint spectrum, called the energy–momentum spectrum.

(1.3) describes however only a finite number of particles in an infinite space. We would like to investigate homogeneous Bose gas at positive density. It is a little problematic how to model such a system. A natural solution would be restricting (1.3) to e.g. $\Lambda = [-L/2, L/2]^d$, the d-dimensional cubic box of side length L, with Dirichlet boundary conditions. This will, however, destroy its translational invariance. Therefore, following the accepted, although somewhat unphysical tradition, we consider the Bose gas on a torus. This means in particular that the potential v is replaced by

$$v^L(\mathbf{x}) = \frac{1}{V} \sum_{\mathbf{k}\in\frac{2\pi}{L}\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\, \hat{v}(\mathbf{k}), \tag{1.4}$$

where $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ is the discrete momentum variable and $V = L^d$ is the volume of the box. 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 on a torus is described by the Hamiltonian

$$H^{L,n} = -\sum_{i=1} \frac{1}{2}\Delta^L_i + \sum_{1\leq i<j\leq n} v^L(\mathbf{x}_i - \mathbf{x}_j) \tag{1.5}$$

acting on the space $L^2_{\mathrm{s}}(\Lambda^n)$ (symmetric square integrable functions on Λ^n). The Laplacian is assumed to have 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 vector of operators

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

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

Clearly, $H^{L,n}$ and $P^{L,n}$ commute with each other. Therefore we can define their joint spectrum

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

which will be called the *energy-momentum spectrum in the box*. By the *excitation spectrum in the box* we will mean $\mathrm{sp}(H^{L,n} - E^{L,n}, P^{L,n})$.

For $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$, we can define the Hamiltonian $H^{L,n}(\mathbf{k})$ to be the restriction of $H^{L,n}$ to the supspace of $P^{L,n} = \mathbf{k}$ and *infimum of the excitation spectrum (IES) in the box* as

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

By the *infimum of the energy-momentum spectrum in the box* we will mean $E^{L,n} + \epsilon^{L,n}(\mathbf{k})$.

It is believed that the properties of the Bose gas simplify in the thermodynamic limit. It means that one should fix $\rho > 0$, take the number of particles equal to $n = \rho V$, and then pass to the limit $L \to \infty$. Unfortunately, as far as we know, the Hamiltonians $H^{L,n} - E^{L,n}$ do not have a limit as self-adjoint operators. One can hope, however, that the IES has some kind of a limit.

Mathematically it is not obvious how to define this limit, since for finite L the IES is defined on the lattice $\frac{2\pi}{L}\mathbb{Z}^d$ and in the thermodynamic limit it should be defined on $\mathbb{R}^d$. Below we propose one of possible definitions of the IES in the thermodynamic limit.

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

$$\epsilon^{\rho}(\mathbf{k}, \delta) := \liminf_{n\to\infty} \left(\inf \left\{ \epsilon^{L,n}(\mathbf{k}') \;:\; \mathbf{k}' \in \frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k} - \mathbf{k}'| < \delta,\ \rho = \frac{n}{L^d} \right\} \right). \tag{1.7}$$

This gives a lower bound on the IES for the momenta $\mathbf{k}'$ 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 in the thermodynamic limit* is defined as its supremum (or, equivalently, its limit) as $\delta \searrow 0$:

$$\epsilon^{\rho}(\mathbf{k}) := \sup_{\delta > 0} \epsilon^{\rho}(\mathbf{k}, \delta). \tag{1.8}$$

Under Assumption (1.1) it is easy to prove that $E^{L,n}$ is finite and $\epsilon^{L,n}(\mathbf{0}) = \epsilon^{\rho}(\mathbf{0}) = 0$ (see Theorem 3.1 and Proposition 3.3).

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

(1) *The function $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon^{\rho}(\mathbf{k}) \in \mathbb{R}_+$ is continuous.*
(2) *Let $\mathbf{k} \in \mathbb{R}^d$. If $L \to \infty$, $n_L \to \infty$, $\frac{n_L}{L^d} \to \rho$, $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$, and $\mathbf{k}_L \to \mathbf{k}$, we have that $\epsilon^{L,n_L}(\mathbf{k}_L) \to \epsilon^{\rho}(\mathbf{k})$.*
(3) *If $d \geq 2$, then $\inf\limits_{\mathbf{k}\neq\mathbf{0}} \frac{\epsilon^{\rho}(\mathbf{k})}{|\mathbf{k}|} =: c_{\mathrm{cr}}^{\rho} > 0$.*
(4) *There exists the limit $\lim\limits_{\mathbf{k}\to\mathbf{0}} \frac{\epsilon^{\rho}(\mathbf{k})}{|\mathbf{k}|} =: c_{\mathrm{ph}}^{\rho} > 0$.*
(5) *The function $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon^{\rho}(\mathbf{k})$ is subadditive, that is, $\epsilon^{\rho}(\mathbf{k}_1 + \mathbf{k}_2) \leq \epsilon^{\rho}(\mathbf{k}_1) + \epsilon^{\rho}(\mathbf{k}_2)$.*

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 $\mathbf{k} = \mathbf{0}$, 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 [3].

(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}^{ρ} will experience no friction. This argument is described e.g. in the course by Landau-Lifshitz [15] and in [41], see also Section 2.6.

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

(3)’ If $d = 1$, then

$$\epsilon^{\rho}(\mathbf{k} + 2\pi\rho) = \epsilon^{\rho}(\mathbf{k}). \tag{1.9}$$

The statement (3)' has a simple rigorous proof, which we will describe in our paper. It implies that in dimension $d = 1$ the excitation spectrum is periodic with the period $2\pi\rho$. It follows by the well known argument that involves boosting all particles simultaneously by the velocity $\frac{2\pi}{L}$ (see e.g. [19]).

Excitation spectrum with the property described by (4) is often described as *phononic* and the excitations with such a spectrum are called *phonons*. One also expects that the parameter c_{ph}^{ρ} coincides with the speed of sound – a parameter in principle macroscopically measurable.

Let us describe a heuristic argument for (5). Suppose that excitations can be described by certain elementary quasiparticles with a dispersion relation $\mathbf{k} \mapsto \omega(\mathbf{k})$. We assume that the state consisting of quasiparticles with momenta $\mathbf{k}_1, \ldots, \mathbf{k}_n$ has the excitation energy $\omega(\mathbf{k}_1) + \cdots + \omega(\mathbf{k}_n)$. Then it is easy to see that the IES is the subadditive hull of $\omega(\mathbf{k})$, that is

$$\epsilon(\mathbf{k}) = \inf\{\omega(\mathbf{k}_1) + \cdots + \omega(\mathbf{k}_n) \ : \ \mathbf{k}_1 + \cdots + \mathbf{k}_n = \mathbf{k}, \quad n = 1, 2, \ldots\}, \tag{1.10}$$

which is the largest subadditive function less than ϵ. In Appendix B we describe a somewhat more elaborate, but still heuristic, argument that seems to indicate that, in the thermodynamic limit, the Bose gas has a subadditive excitation spectrum.

Note that free Bose gas does not satisfy Conjecture 1.1. In this case $\omega(\mathbf{k}) = \frac{1}{2}\mathbf{k}^2$ and $\epsilon(\mathbf{k}) = 0$, see Fig. 1.1.

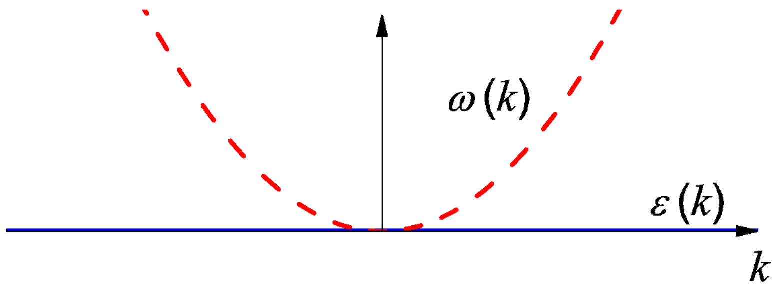

FIGURE 1.1. Excitation spectrum of the free Bose gas

There are not so many subadditive functions. There exist, however, subadditive functions, which satisfy the properties described in our conjecture in (3) or (3)', and in (4). We discuss basic properties of subadditive functions in Appendix A. We could not find these facts in the literature, although they probably belong to the folk knowledge.

1.2. **Critical velocity.** One of the most imporant quantities in in superfluidity is the so-called *critical velocity*. There are several non-equivalent variations of this concept.

One of the variations, which we call the *global* critical velocity, is $\inf_{|\mathbf{k}|} \frac{\epsilon^{L,n}(\mathbf{k})}{|\mathbf{k}|}$. This quantity is responsible for the full *stability* of the superfluid flow, see Subsection 2.6. It plays the role in some physical phenomena, such as the Hess-Fairbank experiment, discussed in [17]. It is positive for the free Bose gas. It is however relevant only in a finite volume, since it vanishes in the thermodynamic limit. To our understanding, it is far too low to account for most other manifestations of superfluidity.

One can also introduce another kind of critical velocity, which we believe is more interesting physically. It can be called the *restricted* critical velocity. In its definition we look first at $\frac{\epsilon^{L,n}(\mathbf{k})}{|\mathbf{k}|}$ for $|\mathbf{k}|$ less then some constant R, then go to the thermodynamic limit, and finally let $R \to \infty$. It is zero for a free Bose gas. If we assume that the dimension $d \geq 2$, the interactions are repulsive and the density is positive, we expect it to be positive in the thermodynamic limit. We believe that it is responsible for the *metastability* of the superfluid flow, see Subsection 2.6.

1.3. **Experimental evidence.** 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 3.4 formulated in the grand-canonical setting) to be true. Let us start with a brief account of experimental evidence for these conjectures.

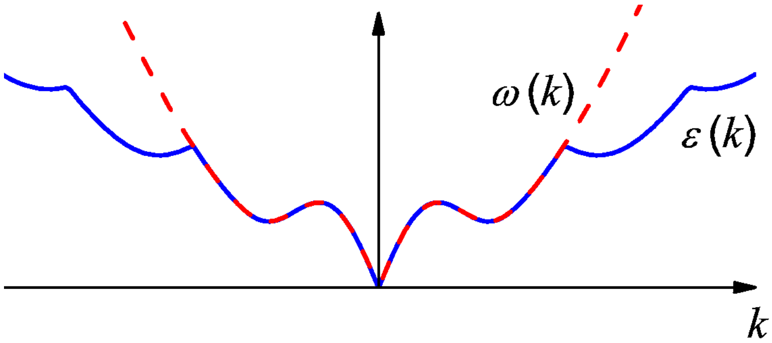

FIGURE 1.2. Excitation spectrum of Helium IV

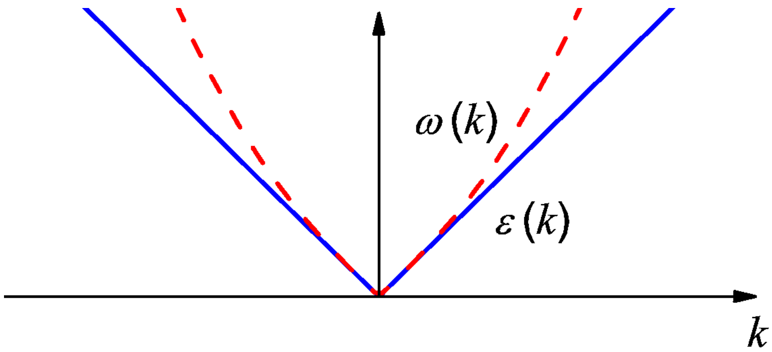

FIGURE 1.3. Excitation spectrum typical for BE condensates of alcalic metals

Theoretically, the cross-section for neutron scattering against a droplet of Helium IV at zero temperature is approximately proportional to the so-called van Hove formfactor $S(\omega, \mathbf{k})$ ([38], see also (H.6)). $S(\omega, \mathbf{k})$ is a measure of the density of excitations of the Bose gas at energy ω and momentum $\mathbf{k}$ at zero temperature. Therefore, $S(\omega, \mathbf{k})$ is zero below the curve $\mathbf{k} \mapsto \epsilon^{\rho}(\mathbf{k})$. It seems reasonable to suppose that more is true: $S(\omega, \mathbf{k})$ should be nonzero everywhere above the curve $\mathbf{k} \mapsto \epsilon^{\rho}(\mathbf{k})$. If in addition Conjecture 1.1 is true, then the lower boundary of the support of $S(\omega, \mathbf{k})$ should satisfy (3), (4) and (5) of this conjecture.

To our understanding, within experimental accuracy, experiments on Helium IV at low temperatures seem to confirm the above theoretical expectations.

Actually, experiments seem to say more than this. At least for low momenta, one observes a sharp peak of $S(\omega, \mathbf{k})$ along a curve similar to $\mathbf{k} \mapsto \omega(\mathbf{k})$ at Fig. 1.2, see [40] and Fig 1 of [24]. This curve is interpreted as the dispersion relation of a quasiparticle (elementary excitation spectrum). These quasiparticles are called phonons for small momenta and rotons around the local minimum of the dispersion relation. To our understanding, experiments indicate that below the subadditive hull of the elementary excitation spectrum the value of $S(\omega, \mathbf{k})$ drops down substantially. (In the case of Fig. 1.2, this subadditive hull equals $\mathbf{k} \mapsto \epsilon(\mathbf{k})$).

Experiments involving excited phonon states are usually successfully interpreted in terms of multi-quasiparticle states whose momenta and energies are additive [24]. This also implies that the energy of multi-quasiparticle states lies above $\mathbf{k} \mapsto \epsilon(\mathbf{k})$.

A similar picture arises in the case of Bose-Einstein (BE) condensates of alcalic metals. For example, the reader can consult Fig. 2 of [33], which shows the quasiparticle spectrum of the BE condensate of ^{87}Rb around zero temperature. Compared to Helium IV, the main difference is the absence of the rotonic part of the elementary excitation spectrum, see Fig. 1.3.

Of course, it is difficult to interpret real experiments in terms of rigorous statements. The setup that we describe in this paper does not apply in all its details to realistic BE condensates. First of all, both in Helium IV and alcalic metals, the potential has typically an attractive part and a hard core. Therefore, strictly speaking it does not belong to the class that we would like to consider in this paper.

In the case of Helium IV, the situation is further complicated by the fact that the Schrödinger operator of the form (1.3) is not believed to describe it adequately – 3-body interactions are probably relevant. This problem does not appear in BE condensates of alcalic metals, where apparently one can assume that only 2-body interactions play the role.

BE condensates of alcalic metals have a different conceptual problem absent in the case of Helium IV: they do not represent the true ground state but only a metastable state.

1.4. **Bogoliubov approximation.** There are many theoretical physics papers devoted to the Bose gas. To our surprise, their authors usually avoid making precise statements or conjectures about the excitation spectrum of the Bose gas. (A notable exception is [41], where a definition of the IES similar to (1.7) can be found).

In [3] Bogoliubov proposed an approximation, which implies that the Bose gas should be described by elementary excitations with the spectrum

$$\omega_{\mathrm{bg}}^{\rho}(\mathbf{k}) = \sqrt{\frac{1}{2}\mathbf{k}^2(\frac{1}{2}\mathbf{k}^2 + 2\hat{v}(\mathbf{k})\rho)}. \tag{1.11}$$

Within this approximation, the IES equals $\epsilon_{\mathrm{bg}}^{\rho}$, the subadditive hull of $\omega_{\mathrm{bg}}^{\rho}$ (see (1.10)), which has the properties described in Conjecture 1.1.

Note that if we replace the potential v with λv and the density ρ with ρ/λ (with a positive λ), then neither $\omega_{\mathrm{bg}}^{\rho}$ nor $\epsilon_{\mathrm{bg}}^{\rho}$ depend on λ. In fact, it is natural to conjecture that $\epsilon_{\mathrm{bg}}^{\rho}$ describes the true IES in the weak coupling–large density limit.

More precisely, let $\epsilon^{\rho,\lambda}(\mathbf{k})$ be the IES for the potential λv.

Conjecture 1.2. *Let $d \geq 2$. Then for a large class of repulsive potentials we have*

$$\lim_{\lambda \searrow 0} \epsilon^{\frac{\rho}{\lambda},\lambda}(\mathbf{k}) = \epsilon_{\mathrm{bg}}^{\rho}(\mathbf{k}).$$

Note that Conjecture 1.2 is certainly wrong in dimension $d = 1$, because of (1.9).

We do not know complete proofs of a statement similar to Conjectures 1.1, 1.2, as well as their grand-canonical analogs described later on in our paper. We believe that to prove or disprove them would be an interesting subject for research in mathematical physics.

Many 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) consider its modifications. They either replace the mode $\mathbf{k} = \mathbf{0}$ by a c-number or drop some of the terms, or do both modifications [1, 14, 9, 11, 36, 42]. These Hamiltonians have no independent justification apart from being approximations to the correct Hamiltonian in some uncontrolled way. Let us stress that in our paper we are mostly interested in the correct Hamiltonian and not its modifications: all our statements will be related either to $H^{L,n}$ or to the grand-canonical Hamiltonian H_μ^L (the second quantization of $H^{L,n} - \mu n$).

1.5. **Organization of the paper.** The paper is divided into several sections and appendices. The individual sections use sometimes slightly different notation and are devoted to different apsects of the Bose gas.

Section 2 is devoted to some facts about Bose gas that are naturally formulated in the canonical approach, where we start with a definite number of particles and go to the thermodynamic limit keeping the density fixed. The later part of the paper, where we use the grand-canonical approach, is independent of this section.

We start with a discussion of the Galileian covariance in a finite box with periodic boundary consitions. We believe that this is relevant if one wants to understand the physics of the Bose gas. Even though what we present is elementary, we did not find most of it in the literature.

In Subsection 2.4 we discuss the case of dimension $d = 1$. We prove that the excitation spectrum is periodic in momentum. This fact is known to some experts and we do not claim its discovery – nevertheless, we have never seen it explicitly stated in the literature.

In Subsection 2.6 we describe an argument that links the properties of the excitation spectrum to superfluid behavior. The argument that we describe is slightly different from the one usually stated in the literature [20, 41] – in particular it applies to systems confined to a finite volume.

In Subsection 2.7 we present the variational ansatz due to Bijls [2] and Feynmann [8] for the excitation spectrum.

In Subsection 2.9 we describe the (non-rigorous but interesting) argument due to Onsager [26] that indicates the phononic character of the excitation spectrum obtained by this ansatz. Our presentation follows that of a recent paper [41].

Section 3 is the central part of our paper. Starting with this section, we switch to the grand-canonical setting. This means that we allow the number of particles to vary and we fix the chemical potential μ. We also use the formalism of second quantization.

In Subsection 3.1 we describe the formalism and formulate Conjecture 3.4, the grand-canonical analog of Conjecture 1.1.

In Subsection 3.2, we discuss the Hamiltonian obtained by a c-number substitution of the mode $\mathbf{k} = \mathbf{0}$. We describe the theorem of Lieb, Seiringer and Yngvason [22] saying that this approximate Hamiltonian gives the correct energy density in the thermodynamic limit. Note that the result of [22] is more general, it concerns an arbitrary temperature. Our presentation sticks to the zero temperature, which allows for some minor simplifications.

In Subsection 3.3 we describe the Bogoliubov approximation. Its original form was formulated in the canonical setting of fixed density in the second-quantized formalism. We follow its grand-canonical version, which can be traced back to Beliaev [1] and Hugenholz - Pines [14], see also a recent review paper by Zagrebnov and Bru [42]. Even though this is a classic reasoning, our presentation seems to be somewhat different from and more satisfactory than what we have seen in the literature. Its first step is a variational problem involving coherent states. The second step is the Bogoliubov translation and rotation adapted to the resulting approximate ground state. Our reasoning does not involve the c-number substitution: we treat the mode $\mathbf{k} = \mathbf{0}$ quantum mechanically.

One can try to improve on Bogoliubov's approximation by looking for the minimum of the energy among translation invariant squeezed states. To our knowledge, in the context of the Bose gas this idea first appeared in the paper of Robinson [31]. 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. In the literature this approach often goes under the name of the Hartree-Fock-Bogoliubov method. One should mention also [6], where a variational bound on the pressure of Bose gas in a positive temperature is derived by using quasi-free states. More recently, similar methods were used to obtain rigorous results about Bose gases in [32, 7].

Only an upper bound to the ground state energy is considered in [31]. 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.

After finding the minimizing squeezed vector Ψ, it is natural to express the Hamiltonian in the new creation/annihilation operators $b_{\mathbf{k}}^*/b_{\mathbf{k}}$, for which the new approximate ground state is a Fock vacuum. We show that the resulting quadratic Hamiltonian has no terms involving b, b^*, bb and b^*b^*. The Hamiltonian becomes

$$H = C + \sum_{\mathbf{k}} D(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}} + \text{terms of order 3 and 4.} \tag{1.12}$$

This new form of the Hamiltonian yields immediately an interesting estimate on the energy-momentum spectrum. In fact, the vectors $b_{\mathbf{k}}^*\Psi$ have precisely the momentum $\mathbf{k}$ and the energy equal to $C + D(\mathbf{k})$. One could ask how good is this estimate. It turns out that it has a serious drawback. As we show in Subsection 3.7, under quite general circumstances we have $D(\mathbf{0}) > 0$.

Perhaps, this is the most important (even if negative) finding of our paper. It implies that at the bottom of its spectrum 1-particle excitations over a squeezed state are poor test functions for the excitation spectrum.

In the literature, the existence of a gap in various approximation schemes that try to improve on the original Bogoliubov's one has been noticed by a number of authors [11, 36]. However, to our knowledge those authors did not consider the correct Hamiltonian, but always used one of its distorted versions.

The Hilbert space of the homogeneous Bose gas can be naturally factorized into the tensor product of an infinite family of Hilbert spaces for various values of the momenta. Variational ansatzes involving translation invariant squeezed states, as well as particle excitations over the squeezed states have a common feature – they are factorized with respect to this tensor product. We call such states *uncorrelated*. One can pose a question: how good are uncorrelated states as variational test functions in many body problems? It seems to us that they have serious drawbacks – in particular, we conjecture that they typically give spectrum with an energy gap.

In Section 4 we discuss approaches to the Bose gas based on perturbation theory. We would like to treat the coupling constant λ as a small parameter, keeping the chemical potential μ fixed.

In Subsection 4.1 we describe a naive splitting of the Hamiltonian into a main part and a perturbation based on the usual Bogoliubov approach. Unfortunately, this approach seems to fail because of a serious infrared problem. We also formulate Conjecture 4.1, which is the grand-canonical analog of Conjecture 1.2 and is suggested by Bogoliubov's approximation.

In Subsection 4.2 we propose a certain systematic procedure for perturbation expansion, which avoids the infrared problem. This procedure uses (1.12) as the starting point for the expansion. The 3rd and 4th order term are treated as perturbations. The advantage of this procedure is that it does not drop any terms from the Hamiltonian. All the works on the Bose gas based on perturbation theory [1, 14, 9] that we know involve the c-number substitution. This substitution, even if justified for the energy density [22], is unfounded for finer quantities such as the infimum of the excitation spectrum. Our perturbative procedure does not involve distorting the Hamiltonian. Therefore, in our opinion, it is superior from the physical point of view.

In Section 5 we describe various inequalities on the Bose gas that can be proved rigorously. These results are consistent with the absence of the energy gap and the phononic form of the excitation spectrum. They are obtained by relatively simple methods, involving especially the so-called f-sum rule. Our presentation is based on the work of Bogoliubov [4] and on results presented by Stringari [34, 35].

In appendices we present some background material, to make our paper accessible to a larger audience. In Appendix F we describe technical computations.

1.6. **Additional remarks about the literature.** Let us make some additional remarks about the literature of the subject. The case of dimension $d = 1$ and repulsive delta interactions has been studied in detail. Girardeau [10] studied the case of "infinite" coupling (which amounts to the Dirichlet boundary conditions). The case of an arbitrary positive coupling constant was studied in [20, 19], where arguments for the absence of a gap and the phononic shape of the excitation spectrum in the thermodynamic limit are given. [41] gives a full rigorous proof for the linearity of the excitation spectrum in the thermodynamic limit for Girardeau's model. Note, however, that the 1-dimensional case is believed to be quite different from the case $d \geq 2$.

There exists a large literature on the energy density of the Bose gas. The energy density can be defined as

$$e^\rho := \lim_{L\to\infty} \frac{E^{L,n}}{V}, \tag{1.13}$$

where $\rho = \frac{n}{V}$ is kept fixed. There exist derivations of the asymptotics of e^ρ in dimension $d = 3$ for small ρ going back to [5, 14, 16, 18]. This asymptotics is not restricted to small potentials – it covers also the case of hard-core potentials. One can show rigorously (see [23] and references therein) that the leading term of this asymptotics correctly describes the energy density. Similar results can be shown in dimension $d = 2$.

Note that the energy density is easier to study than the infimum of the excitation spectrum. Besides, it does not capture some interesting physical phenomena the excitation spectrum is responsible for. Note also that the above mentioned results involve the following limit: the scattering length is kept fixed (this can be achieved e.g. by fixing the potential) and the density goes to zero. In our paper we usually consider a different limit: the chemical potential is kept fixed and the coupling constant in front of the potential goes to zero. One can have various opinions comparing the physical relevance of the two limits. In any case, the latter limit seems more appropriate if one wants to capture the phononic character of the excitation spectrum.

Another direction of rigorous research involves studying the so-called Gross-Pitaevski limit. Again it concerns mostly the dimension $d = 3$. The quantity that is kept fixed is $\frac{an}{L}$, where a is the scattering length and n goes to infinity. The Gross-Pitaevski limit is usually presented with a fixed L and the scattering length a going to zero, which is achieved by an appropriate scaling of the potential.

Equivalently, one can fix the potential, consider $L \to \infty$. and scale the density as $\rho \sim L^{1-d}$ as $L \to \infty$. In this limit, Lieb, Seiringer and Yngvason have obtained a number of interesting and precise results [23]. In particular, they are able to approximate the behavior of the n-body system by a non-linear effective equation – the Gross-Pitaevski equation. Note, however, that in this limit it is difficult to say something interesting about the excitation spectrum, because the density, and hence the speed of sound and the critical velocity, go to zero.

The result of [21] (see also Theorem 5.3 of [23]) can be interpreted as the positivity of the *global* critical velocity in finite volume. This result does not address the properties of the *restricted* critical velocity.

Finally, let us note that there exists a number of interesting rigorous results about Bose gas in positive temperatures [4, 6, 13, 34, 35, 27, 22].

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2. Canonical approach

In this section we will always work on a Hilbert space of fixed number of particles. We will use the Hamiltonian $H^{L,n}$ introduced in the introduction. To simplify the notation, we often drop the superscripts n, L, writing e.g. H instead of $H^{L,n}$.

2.1. **Free Bose gas.** In finite volume, the momentum is restricted to

$$\mathbf{k} = \frac{2\pi}{L}\tilde{\mathbf{k}}, \quad \tilde{\mathbf{k}} \in \mathbb{Z}^d.$$

It is easy to compute exactly the excitation spectrum of the free Bose gas in a finite volume, see Fig 2.1. In particular, in dimension $d = 1$, its infimum is given by the broken line with vertices at

$$\mathbf{k} = \frac{2\pi n}{L}\tilde{\mathbf{k}}, \quad \epsilon^{L,n}(\mathbf{k}) = \frac{1}{2}\mathbf{k}^2, \qquad \tilde{\mathbf{k}} \in \mathbb{Z}.$$

In an arbitrary dimension, we just add the contributions from each dimension:

$$\epsilon^{L,n}(\mathbf{k}_1, \dots, \mathbf{k}_d) = \epsilon^{L,n}(\mathbf{k}_1) + \cdots + \epsilon^{L,n}(\mathbf{k}_d).$$

2.2. **Galileian covariance in a box with periodic boundary conditions.**

In infinite volume the Galileian covariance involves an arbitrary value of velocity. This is not the case in a box with periodic boundary conditions (torus), where the Galileian covariance is only rudimentary. To describe it we will restrict ourselves to boosts in the first coordinate. The following operator, which we will call the *boost operator*, adds simultaneously velocity $\frac{2\pi}{L}$ to all particles in the direction of the first coordinate:

$$U_1 := \exp\left(\frac{\mathrm{i}2\pi}{L}\sum_{i=1}^{n}\mathbf{x}_{i1}\right).$$

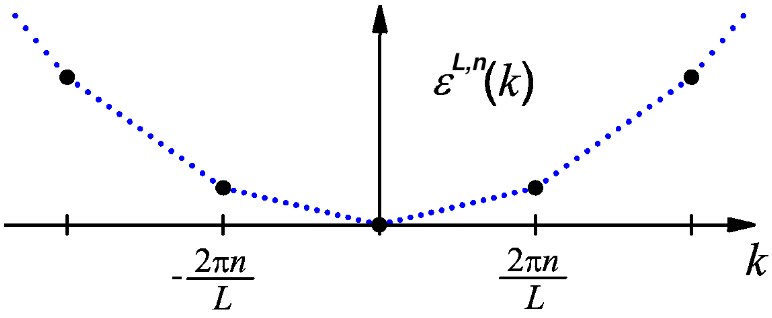

FIGURE 2.1. Infimum of excitation spectrum of free Bose gas in finite volume

($\mathbf{x}_{i1}$ denotes the 1st coordinate of the ith particle). Clearly, U_1 preserves the domain of H and is a unitary operator on $L_{\mathrm{s}}(\Lambda^n)$ satisfying

$$U_1 P_1 U_1^* = P_1 - \frac{2\pi n}{L}, \tag{2.1}$$

$$U_1 H U_1^* = H - \frac{2\pi}{L} P_1 + \frac{(2\pi)^2 n}{2L^2}. \tag{2.2}$$

(P_1 denotes the first component of the total momentum). Hence

$$U_1 \left(H - \frac{1}{2n} P^2 \right) U_1^* = H - \frac{1}{2n} P^2. \tag{2.3}$$

(2.3) and (2.2) imposes a severe restriction on the shape of the excitation spectrum:

$$\mathrm{sp} \left(H - \frac{1}{2n} P^2 \right) \tag{2.4}$$

has to be invariant with respect to translations by $\frac{2\pi n}{L}$, see Fig. 2.2.

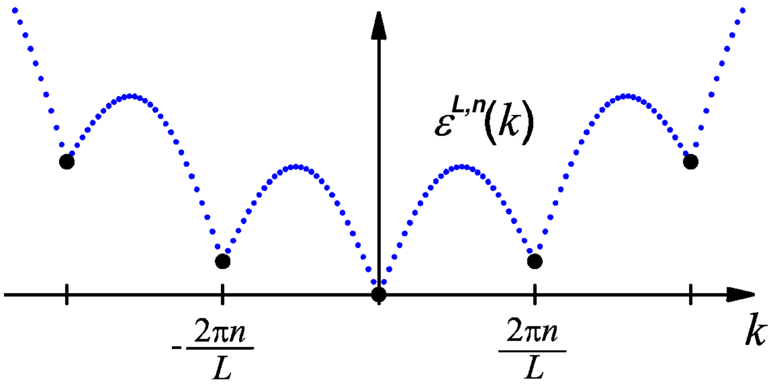

FIGURE 2.2. Typical infimum of excitation spectrum of interacting Bose gas in finite volume

2.3. **Critical velocity.** The global critical velocity in finite volume is defined by

$$c_{\mathrm{cr}}^{L,n} := \inf_{\mathbf{k} \neq \mathbf{0}} \frac{\epsilon^{L,n}(\mathbf{k})}{|\mathbf{k}|}.$$

Recall that we are interested in the thermodynamic limit, which involves $L, n \to \infty$ with $\frac{n}{V} = \rho > 0$.

Note that for the free Bose gas we have

$$c_{\mathrm{cr}}^{L,n} = \frac{\pi}{L}. \tag{2.5}$$

Thus the global critical velocity is positive, but goes to zero in the thermodynamic limit.

In the interacting case we have a sequence of low energy states with the momentum and the excitation energy obtained by boosting the ground state:

$$\mathbf{k} = \frac{2\pi n}{L}\tilde{\mathbf{k}}, \quad \epsilon = \frac{(2\pi)^2}{2L^2} n\tilde{\mathbf{k}}^2.$$

where $\tilde{\mathbf{k}} \in \mathbb{Z}^d$. Expressed in terms of density this gives

$$\mathbf{k} = 2\pi\rho L^{d-1}\tilde{\mathbf{k}}, \quad \epsilon = \frac{(2\pi)^2}{2}\rho L^{d-2}\tilde{\mathbf{k}}^2,$$

Therefore, in the general case the global critical velocity is not greater than in the case of the free gas:

$$c_{\mathrm{cr}}^{L,n} \leq \frac{\pi}{L}.$$

In dimension $d \geq 2$, the momentum of these states escapes to infinity, so in a sense they are not visible in the thermodynamic limit.

2.4. **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)', that is

Theorem 2.1. $\mathbb{R} \ni \mathbf{k} \mapsto \epsilon^\rho(\mathbf{k})$ *is periodic with the period* $2\pi\rho$.

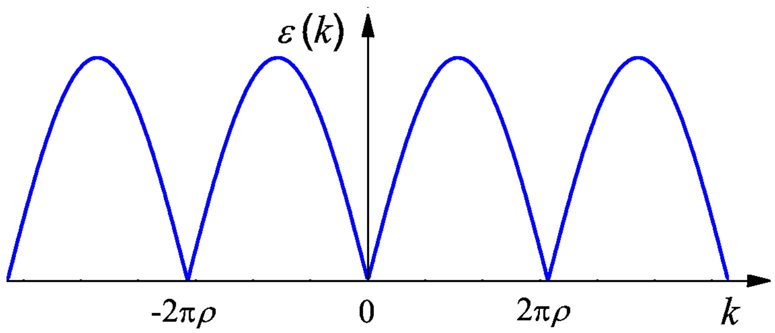

FIGURE 2.3. Typical infimum of excitation spectrum of Bose gas in dimension $d = 1$

Theorem 2.1 easily follows from the invariance of the spectrum (2.4).

2.5. **Twisted boundary conditions.** One can also consider the boost operator for an arbitrary velocity. In fact, for $\alpha \in \mathbb{R}$, define the unitary operator

$$U_1(\alpha) := \exp\left(\frac{\mathrm{i}\alpha}{L}\sum_{i=1}^{n} \mathbf{x}_{i1}\right).$$

Let $[\alpha]$ denote $\alpha \mod (2\pi)$. We will write $P_{1,[\alpha]}$, $H_{[\alpha]}$ for the momentum and the Hamiltonian with the boundary condition in the 1st coordinate twisted by $[\alpha]$. (It means that the elements of the domain of these operators for $j = 1, \ldots, n$ satisfy

$$\Phi\left(\mathbf{x}_1, \ldots, \mathbf{x}_j - \frac{1}{2}L\,\mathrm{e}_1, \ldots, \mathbf{x}_n\right) = \mathrm{e}^{\mathrm{i}\alpha}\,\Phi\left(\mathbf{x}_1, \ldots, \mathbf{x}_j + \frac{1}{2}L\,\mathrm{e}_1, \ldots, \mathbf{x}_n\right),$$

where e_1 is the unit vector in the direction of the 1s coordinate).

For α not equal to a multiple of 2π the operator $U_1(\alpha)$ does not preserve the domain of H and P. Instead of identities (2.1) and (2.2) we have

$$\begin{aligned} U_1(\alpha)P_1U_1(-\alpha) &= P_{1,[\alpha]} - \frac{\alpha n}{L}, && (2.6)\\ U_1(\alpha)HU_1(-\alpha) &= H_{[\alpha]} - \frac{\alpha}{L}P_{1,[\alpha]} + \frac{\alpha^2 n}{2L^2}, && (2.7) \end{aligned}$$

(2.6) and (2.7) imply

$$H_{[\alpha]} = U_1(\alpha)\left(H + \frac{\alpha}{L}P_1\right)U_1(-\alpha) + \frac{\alpha^2 n}{2L^2}. \tag{2.8}$$

In particular, if $0 \leq \alpha_0 \leq \pi$, then

$$c_{\rm cr}^{L,n} \geq \frac{\alpha_0}{L}$$

if and only if

$$H_{[\alpha]} - E \geq \frac{\alpha^2 n}{2L^2}, \quad |\alpha| \leq \alpha_0. \tag{2.9}$$

(2.9) was used by Lieb, Seiringer and Yngvason as a criterion for the positivity of global critical velocity in [21], see also Theorem 5.3 of [23].

2.6. **Superfluidity.** Let us describe one of experiments that show superfluid properties of the Bose gas.

A laser beam playing the role of an optical spoon [30] is directed into a sample of a Bose gas at a sufficiently low temperature. The beam makes a rotating motion. If the velocity of this motion is lower than a certain critical value, then the sample heats up very slowly. For velocities above this critical value, the sample heats up much faster.

Let us try to describe an idealized mathematical model of this phenomenon, which is a version of the well known argument due to Landau described e.g. in [15, 41].

Since our Bose gas has periodic boundary conditions, we can make an idealized assumption that the "laser beam" travels forever with a constant velocity $\mathbf{w} = (w, 0, \dots, 0) \in \mathbb{R}^d$. We will model it with a weak travelling potential $u(\mathbf{x} - t\mathbf{w})$ interacting with all particles. Thus the system is described by the Schrödinger equation with a time-dependent Hamiltonian

$$\mathrm{i}\partial_t \Psi_t = \left(H + \sum_{i=1}^n u(\mathbf{x}_i - t\mathbf{w})\right)\Psi_t. \tag{2.10}$$

Let us replace Ψ_t with

$$\tilde{\Psi}_t(\mathbf{x}_1, \dots, \mathbf{x}_n) := \Psi_t(\mathbf{x}_1 + t\mathbf{w}, \dots, \mathbf{x}_n + t\mathbf{w}).$$

We obtain a Schrödinger equation with a time-independent Hamiltonian:

$$\mathrm{i}\partial_t \tilde{\Psi}_t = \left(H - \mathbf{w}P + \sum_{i=1}^n u(\mathbf{x}_i)\right)\tilde{\Psi}_t.$$

We know that the operator H has a nondegenerate ground state energy E. The corresponding ground state Ψ is therefore stable with respect to small time-independent perturbations. We ask the question whether the state Ψ is stable against a small travelling perturbation of the form (2.10).

Let us first describe a slightly dishonest version of the argument for superfluidity (which actually is usually found in the literature). Let $c_{\rm cr}$ denote the critical velocity. For $|\mathbf{w}| < c_{\rm cr}$, the excitation spectrum of the "tilted Hamiltonian" $H - \mathbf{w}P$ looks as at Fig. 2.4, so Ψ is its ground state. Hence Ψ hence is stable. For $|\mathbf{w}| > c_{\rm cr}$ the excitation spectrum looks as at Fig. 2.5. Therefore Ψ is not a ground state

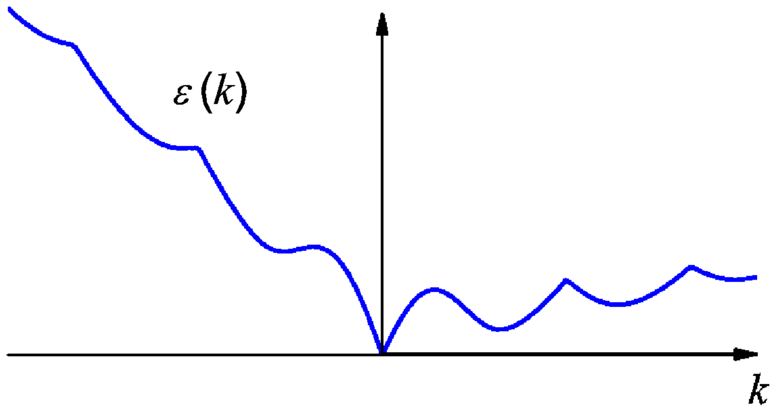

FIGURE 2.4. Infimum of excitation spectrum of tilted Hamiltonian for velocity below c_{cr}

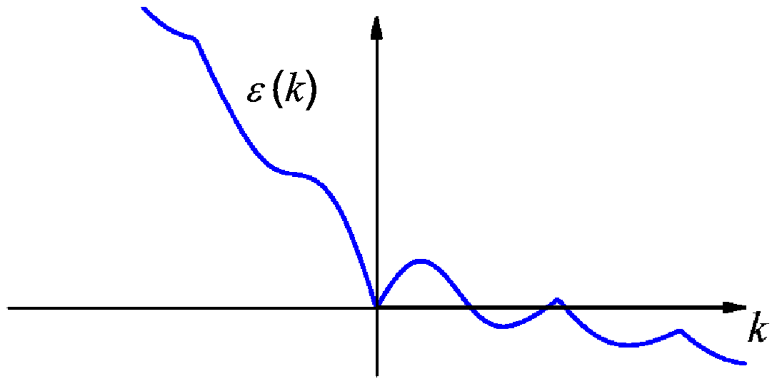

FIGURE 2.5. Infimum of excitation spectrum of tilted Hamiltonian for velocity above c_{cr}

of $H - \mathbf{w}P$ and its energy is close to energies of many other states. Hence Ψ is unstable.

Note that we cheated a little in the above argument. The situation that we described involved a finite volume, but the pictures were (as we believe) typical for the thermodynamic limit. The actual plot in finite volume resembles Figure 2.6. In particular the global critical velocity in finite volume $c_{\mathrm{cr}}^{L,n}$ is small and goes to zero in the thermodynamic limit. Physical evidence seems to indicate that the superfluid flow can be metastable at much larger velocities, which are positive in the thermodynamic limit. Note that the Figs 2.4 and 2.5 represent the excitation spectrum in the thermodynamic limit and do not show the low lying states present in finite volume, which have a very low critical velocity.

Let us try to present a more physical argument for superfluidity. Suppose that the Fourier transform of u is supported in the ball $|\mathbf{k}| \leq R$. Define the *restricted critical velocity below the momentum* R as

$$c_{\mathrm{cr},R}^{L,n} := \inf \left\{ \frac{\epsilon^{L,n}(\mathbf{k})}{|\mathbf{k}|} \quad \mathbf{k} \neq \mathbf{0}, \quad |\mathbf{k}| < R \right\}. \tag{2.11}$$

If the "tilted Hamiltonian" $H^{L,n} - \mathbf{w}P^{L,n}$ has no other eigenstates of energy close to $E^{L,n}$ and momentum less that R, then the state Ψ will be metastable against the perturbation (2.10), at least in the 1st order. This is the case for $|\mathbf{w}| < c_{\mathrm{cr},R}^{L,n}$.

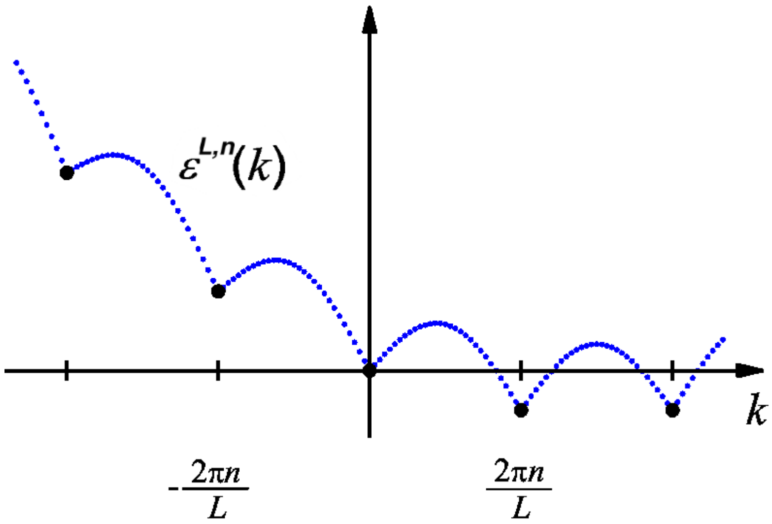

FIGURE 2.6. Infimum of excitation spectrum of "tilted Hamiltonian" in finite volume

On the other hand, for $|\mathbf{w}| \geq c_{\mathrm{cr},R}^{L,n}$, we can expect many states with energy close to $E^{L,n}$ and momentum less than R, so the metastability will be lost.

Heuristic arguments (e.g. the Bogoliubov method described later on) suggest that in dimension $d \geq 2$, for a positive density ρ and for an arbitrary R, the restricted critical velocity $c_{\mathrm{cr},R}^{L,n}$ is bounded away from zero even in the thermodynamic limit. This can be formulated in the following conjecture:

Conjecture 2.2. *Fix density ρ. Then*

$$c_{\mathrm{cr},R}^{\rho} := \lim_{L\to\infty} c_{\mathrm{cr},R}^{L,n}, \quad \frac{n}{V} = \rho,$$

exists, where $c_{\mathrm{cr},R}^{L,n}$ is defined as in (2.11). Moreover, in dimension $d \geq 2$,

$$\liminf_{R\to\infty} c_{\mathrm{cr},R}^{\rho} > 0. \tag{2.12}$$

We think that the statement of Conjecture 2.2, and in particular (2.12), is a good candidate for the *definition of superfluidity at zero temperature*. Another candidate for a such definiton is the statement of Conjecture 1.1 (3).

Note in parenthesis, that Conjecture 2.2 is stronger than Conjecture 1.1 (3). In fact, the left hand side of (2.12) is less than or equal to c_{cr}^{ρ} introduced in Conjecture 1.1 (3).

2.7. **Bijls–Feynmann's ansatz.** For $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ set

$$N_{\mathbf{k}} := \sum_{i=1}^{n} \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}_i}, \tag{2.13}$$

acting on $L_{\mathrm{s}}^2(\Lambda^n)$.

It is well known that the ground state of H is nondegenerate. Denote it by Ψ. We will write (see Appendix G)

$$\langle A \rangle := (\Psi|A\Psi), \qquad \langle\langle A, B \rangle\rangle := \langle A(H-E)^{-1}B\rangle + \langle B(H-E)^{-1}A\rangle.$$

Note the following identity:

$$\frac{1}{2}[N_{\mathbf{k}}^*,[H,N_{\mathbf{k}}]]=\frac{\mathbf{k}^2}{2}n. \tag{2.14}$$

It implies the so called *f-sum rule*:

$$\frac{1}{2}\langle N_{\mathbf{k}}^*(H-E)N_{\mathbf{k}}\rangle+\frac{1}{2}\langle N_{\mathbf{k}}(H-E)N_{\mathbf{k}}^*\rangle=\frac{\mathbf{k}^2}{2}n. \tag{2.15}$$

By the reality of Ψ and H, (2.15) also equals $\langle N_{\mathbf{k}}^*(H-E)N_{\mathbf{k}}\rangle$. Define

$$\begin{aligned} s_{\mathbf{k}} &:= n^{-1}\langle N_{\mathbf{k}}^*N_{\mathbf{k}}\rangle; && (2.16)\\ \chi_{\mathbf{k}} &:= n^{-1}\langle\langle N_{\mathbf{k}}^*,N_{\mathbf{k}}\rangle\rangle. && (2.17)\end{aligned}$$

By the reality of Ψ and H, (2.17) also equals $2n^{-1}\langle N_{\mathbf{k}}^*(H-E)^{-1}N_{\mathbf{k}}\rangle$.

By the Schwarz inequality, we obtain

$$s_{\mathbf{k}}\leq\frac{1}{2}|\mathbf{k}|\sqrt{\chi_{\mathbf{k}}}. \tag{2.18}$$

Bijls [2] and Feynmann [8] proposed to consider the following variational ansatz:

$$\Psi_{\mathbf{k}}:=N_{\mathbf{k}}\Psi/\|N_{\mathbf{k}}\Psi\|,$$

to obtain the excitation spectrum of the Bose gas.

Theorem 2.3. *We have*

$$\begin{aligned} P\Psi_{\mathbf{k}} &= \mathbf{k}\Psi_{\mathbf{k}}, && (2.19)\\ \Psi_{\mathbf{0}} &= \Psi, && (2.20)\\ (\Psi_{\mathbf{k}}|(H-E)\Psi_{\mathbf{k}}) &= \frac{|\mathbf{k}|^2}{2s_{\mathbf{k}}}\geq\frac{|\mathbf{k}|}{\sqrt{\chi_{\mathbf{k}}}}. && (2.21)\end{aligned}$$

Proof. To see (2.21) we note that

$$\begin{aligned}(\Psi_{\mathbf{k}}|(H-E)\Psi_{\mathbf{k}}) &= \frac{\langle N_{\mathbf{k}}^*(H-E)N_{\mathbf{k}}\rangle+\langle N_{\mathbf{k}}(H-E)N_{\mathbf{k}}^*\rangle}{2\langle N_{\mathbf{k}}^*N_{\mathbf{k}}\rangle}\\ &= \frac{\mathbf{k}^2}{2s_{\mathbf{k}}}\geq\frac{|\mathbf{k}|}{\sqrt{\chi_{\mathbf{k}}}},\end{aligned}$$

where we applied the f-sum rule to the numerator and used (2.18). □

It is believed that the Bijls-Feynman ansatz gives the correct behavior of the excitation spectrum for low momenta, and in particular it gives the value of c_{ph}^{ρ}, which was defined in Conjecture 2.2 (4) [35]. Let us formulate this as a conjecture:

Conjecture 2.4. *Fix density ρ. Let $\mathbb{R}^d\ni\mathbf{k}\mapsto\epsilon_{\mathrm{BF}}^{\rho}(\mathbf{k})$ be defined as in (1.7) and (1.8) with $(\Psi_{\mathbf{k}}|(H^{L,n}-E^{L,n})\Psi_{\mathbf{k}})$ replacing $\epsilon^{L,n}(\mathbf{k})$. (In other words, $\epsilon_{\mathrm{BF}}^{\rho}(\mathbf{k})$ is a thermodynamic limit of the left hand side of (2.21)). Then*

$$\lim_{\mathbf{k}\to\mathbf{0}}\frac{\epsilon^{\rho}(\mathbf{k})}{|\mathbf{k}|}=\lim_{\mathbf{k}\to\mathbf{0}}\frac{\epsilon_{\mathrm{BF}}^{\rho}(\mathbf{k})}{|\mathbf{k}|}. \tag{2.22}$$

2.8. **Speed of sound.** Recall that under broad conditions we are able to prove the existence of the energy density (1.13), which for typographical reasons in this subsection we will be written $e(\rho)$ instead of e^{ρ}.

Another important macroscopic parameter, which in principle can be measured experimentally, is the speed of sound, denoted c_{s}. It is related to the energy density by

$$c_{\mathrm{s}}=\sqrt{\rho e''(\rho)} \tag{2.23}$$

(see e.g. Appendix C).

It is believed that for low momenta

$$\lim_{\mathbf{k}\to\mathbf{0}} \frac{s_{\mathbf{k}}}{|\mathbf{k}|} = \frac{1}{2c_{\mathrm{s}}}, \tag{2.24}$$

and hence $(\Psi_{\mathbf{k}}|(H-E)\Psi_{\mathbf{k}}) \sim c_{\mathrm{s}}|\mathbf{k}|$. If this is the case and if the speed of sound is nonzero, then the excitation spectrum given by the Bijls-Feynman ansatz is phononic, that is the limit on the right hand side of (2.22) exists and equals c_{s}.

2.9. **Relation between the speed of sound and $\chi_{\mathbf{k}}$.** Instead of arguing for (2.24), it seems easier to justify the relation

$$\lim_{\mathbf{k}\to\mathbf{0}} \chi_{\mathbf{k}} = \frac{1}{c_{\mathrm{s}}^2} \tag{2.25}$$

In this subsection we describe a series of heuristic arguments indicating that (2.25) holds in the thermodynamic limit. Given (2.25) and if the speed of sound is nonzero, (2.21) gives a phononic lower bound on $(\Psi_{\mathbf{k}}|(H-E)\Psi_{\mathbf{k}})$. This inequality is attributed to Onsager [26]. Our presentation follows that of [41].

Let $C^\infty_{\mathrm{per}}(\mathbb{R}^d)$ denote the set of smooth periodic functions. If $u \in C^\infty_{\mathrm{per}}(\mathbb{R}^d)$, we will often identify it with its restriction to Λ, where we assume that L is a multiple of the period of u. We also introduce a notation for the perturbed Hamiltonian

$$H_u := H + \sum_i u(\mathbf{x}_i). \tag{2.26}$$

We denote by E_u the ground state energy of H_u. We also set

$$E_u^{\mathrm{df}} := \inf \int_\Lambda \left(e(\varrho(\mathbf{x})) + u(\mathbf{x})\varrho(\mathbf{x})\right) \mathrm{d}\mathbf{x},$$

where we take the infimum over positive functions $\Lambda \ni \mathbf{x} \mapsto \varrho(\mathbf{x})$ satisfying $\int_\Lambda \varrho(\mathbf{x})\mathrm{d}\mathbf{x} = n$. (The superscript df stands for the *density functional*).

Let F be a function depending on $u \in C^\infty_{\mathrm{per}}(\mathbb{R}^d)$. We will say that $F(u) = o(|\nabla u|^0)$ iff there exists N and a function f such that $\lim\limits_{\tau\to 0} f(\tau) = 0$ and

$$|F(u)| \quad \leq \quad f\left(\sum_{1\leq|\alpha|\leq N} \sup |\partial^\alpha_{\mathbf{x}} u(\mathbf{x})|\right),$$

Conjecture 2.5. *E_u^{df} is an approximation of E_u for slowly varying u, more precisely,*

$$\limsup_{L\to\infty,\quad n=\rho V} \frac{1}{V}\left|E_u - E_u^{\mathrm{df}}\right| \quad = \quad o(|\nabla u|^0).$$

The next claim follows from Conjecture (2.5) by an application of a perturbation argument:

Conjecture 2.6. *For $u \in C^\infty_{\mathrm{per}}(\mathbb{R}^d)$ having the mean value equal to zero we have*

$$\left|\frac{1}{Ve''(\rho)}\int u(\mathbf{x})^2 \mathrm{d}\mathbf{x} - \frac{2}{V}\left\langle \sum_i u(\mathbf{x}_i)(H-E)^{-1}\sum_i u(\mathbf{x}_i)\right\rangle\right| \quad = \quad o(|\nabla u|^0).$$

Let us give an argument in favor of Conjecture 2.6. For $\tau \in \mathbb{R}$, we consider the family of Hamiltonians $H_{\tau u}$ with the ground state energy $E_{\tau u}$. By the usual perturbation theory,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}(E_{\tau u}-E) &= 0, && (2.27)\\
\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}(E_{\tau u}-E) &= -2\left\langle \sum_i u(\mathbf{x}_i)(H-E)^{-1}\sum_i u(\mathbf{x}_i)\right\rangle. && (2.28)
\end{aligned}$$

Now

$$\begin{aligned}
E^{\mathrm{df}}_{\tau u} &= \inf\left\{\int e(\varrho(\mathbf{x}))\mathrm{d}\mathbf{x}+\tau\int\varrho(\mathbf{x})u(\mathbf{x})\mathrm{d}\mathbf{x}\right\} && (2.29)\\
&\approx Ve(\rho)\\
&\quad+\inf\left\{\int\frac{e''(\rho)}{2}(\varrho(\mathbf{x})-\rho)^2\mathrm{d}\mathbf{x}+\tau\int(\varrho(\mathbf{x})-\rho)u(\mathbf{x})\mathrm{d}\mathbf{x}\right\}, && (2.30)
\end{aligned}$$

where in (2.29) and (2.30) we minimize over positive functions ϱ such that $\int\varrho(\mathbf{x})\mathrm{d}\mathbf{x}=n$. The minimum of (2.30) is attained at

$$\varrho(\mathbf{x}) := \rho-\frac{\tau}{e''(\rho)}u(\mathbf{x}).$$

Therefore,

$$E^{\mathrm{df}}_{\tau u} \approx Ve(\rho)-\int\frac{\tau^2}{2e''(\rho)}u(\mathbf{x})^2\mathrm{d}\mathbf{x}.$$

Invoking (2.28) we obtain Conjecture 2.6.

Now (2.25) will follow from (2.23) and the following claim:

Conjecture 2.7. $\chi_{\mathbf{k}}$ *is well defined in the thermodynamic limit and satisfies*

$$\lim_{\mathbf{k}\to\mathbf{0}}\chi_{\mathbf{k}}=\frac{1}{e''(\rho)\rho}. \qquad (2.31)$$

Let us justify (2.31). We assume that L is large. Clearly,

$$\begin{aligned}
\langle N^*_{\mathbf{k}}(H-E)^{-1}N_{\mathbf{k}}\rangle &= \left\langle\sum_i\cos(\mathbf{k}\mathbf{x}_i)(H-E)^{-1}\sum_j\cos(\mathbf{k}\mathbf{x}_j)\right\rangle\\
&\quad+\left\langle\sum_i\sin(\mathbf{k}\mathbf{x}_i)(H-E)^{-1}\sum_j\sin(\mathbf{k}\mathbf{x}_j)\right\rangle\\
&\quad+2\mathrm{Im}\left\langle\sum_i\sin(\mathbf{k}\mathbf{x}_i)(H-E)^{-1}\sum_j\cos(\mathbf{k}\mathbf{x}_j)\right\rangle. \qquad (2.32)
\end{aligned}$$

The ground state Ψ is a real vector. The Hamiltonian H, and hence also $(H-E)^{-1}$, is a real operator. Therefore, the last term in (2.32) is zero.

Obviously,

$$\frac{1}{Ve''(\rho)}\int(\cos^2(\mathbf{k}\mathbf{x})+\sin^2(\mathbf{k}\mathbf{x}))\mathrm{d}\mathbf{x} = \frac{1}{e''(\rho)}.$$

Hence, by Conjecture 2.6,

$$\lim_{\mathbf{k}\to\mathbf{0}}\limsup_{L\to\infty,\ n=\rho V}\left|\frac{2}{V}\langle N^*_{\mathbf{k}}(H-E)^{-1}N_{\mathbf{k}}\rangle-\frac{1}{e''(\rho)}\right|=0,$$

which implies (2.31).

3. Bogoliubov approach in the grand-canonical setting

3.1. **Grand-canonical approach to the Bose gas.** As realized by Bogoliubov [3], even if one is interested in properties of the Bose gas with a fixed but large number of particles, it is convenient to use the second quantized description of the system, allowing for an arbitrary number of particles.

An additional reformulation of the problem was noted already by Beliaev [1], Hugenholz - Pines [14] and others. Instead of studying the Bose gas in the canonical formalism, fixing the density, it is mathematically more 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 $\mu \geq 0$ on the symmetric Fock space

$$\Gamma_{\mathrm{s}}(L^2(\Lambda)) := \mathop{\oplus}_{n=0}^{\infty} L^2_{\mathrm{s}}(\Lambda^n),$$

we define the grand-canonical Hamiltonian

$$\begin{aligned} H^L_\mu &:= \mathop{\oplus}_{n=0}^{\infty} \left(H^{L,n} - \mu n\right) \\ &= \int a^*_{\mathbf{x}}(-\frac{1}{2}\Delta_{\mathbf{x}} - \mu)a_{\mathbf{x}}\mathrm{d}\mathbf{x} + \frac{1}{2}\int\int a^*_{\mathbf{x}}a^*_{\mathbf{y}}v^L(\mathbf{x}-\mathbf{y})a_{\mathbf{y}}a_{\mathbf{x}}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}. \end{aligned}$$

The second quantized momentum and number operators are defined as

$$\begin{aligned} N^L &:= \mathop{\oplus}_{n=0}^{\infty} n = \int a^*_{\mathbf{x}}a_{\mathbf{x}}\mathrm{d}\mathbf{x}, \\ P^L &:= \mathop{\oplus}_{n=0}^{\infty} P^{n,L} = -\mathrm{i}\int a^*_{\mathbf{x}}\nabla^L_{\mathbf{x}}a_{\mathbf{x}}\mathrm{d}\mathbf{x}. \end{aligned}$$

It is convenient to pass to the momentum representation:

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

where we used (1.4) 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 $a_{\mathbf{x}} = V^{-1/2}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}}\, a_{\mathbf{k}}$.

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

$$E^L_\mu = \inf \mathrm{sp} H^L_\mu = \inf_{n\geq 0}(E^{L,n} - \mu n). \tag{3.1}$$

E^L_μ is a decreasing concave function of μ. To go back to the canonical condition (fixed number of particles) one uses

$$n \;=\; -\partial_\mu E^L_\mu. \tag{3.2}$$

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

Theorem 3.1. *Suppose that $\hat{v}(\mathbf{k}) \geq 0$, $\hat{v}(\mathbf{0}) > 0$ and $v(\mathbf{0}) < \infty$. Then $H^{L,n}$ and H_μ^L are bounded from below and*

$$E^{L,n} \geq \frac{\hat{v}(\mathbf{0})}{2V}n^2 - \frac{v(\mathbf{0})}{2}n, \tag{3.3}$$

$$E_\mu^L \geq -V\frac{(\frac{1}{2}v(\mathbf{0}) + \mu)^2}{2\hat{v}(\mathbf{0})}. \tag{3.4}$$

Proof. Let us drop the subscript L. Set

$$N_{\mathbf{q}} := \sum_{\mathbf{k}} a_{\mathbf{k}+\mathbf{q}}^* a_{\mathbf{k}} = \int \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}}\, a_{\mathbf{x}}^* a_{\mathbf{x}} \mathrm{d}\mathbf{x}, \tag{3.5}$$

(which is the second quantized version of (2.13)). Then, by a simple commutation, using that $N_{\mathbf{0}} = N$ and that $\hat{v}(\mathbf{k})$ is non-negative, we obtain

$$\begin{aligned} H_\mu &\geq -\mu N + \frac{1}{2V}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\hat{v}(\mathbf{k}_2 - \mathbf{k}_3) a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4} \\ &= \frac{1}{2V}\sum_{\mathbf{k}} \hat{v}(\mathbf{k}) N_{\mathbf{k}}^* N_{\mathbf{k}} - (\mu + \frac{v(\mathbf{0})}{2})N \\ &\geq \frac{\hat{v}(\mathbf{0})}{2V}N^2 - (\mu + \frac{v(\mathbf{0})}{2})N. \end{aligned} \tag{3.6}$$

Setting $\mu = 0$ and $N = n$ in (3.6) we obtain (3.3). Minimizing (3.6) over N proves (3.4). □

For $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ let $H_\mu^L(\mathbf{k})$ denote the Hamiltonian H_μ^L restricted to the space $P = \mathbf{k}$. The *IES in the box* is defined as

$$\epsilon_\mu^L(\mathbf{k}) := \inf \mathrm{sp} H_\mu^L(\mathbf{k}). \tag{3.7}$$

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

$$\epsilon_\mu(\mathbf{k}) := \sup_{\delta>0}\left(\liminf_{L\to\infty}\left(\inf_{\mathbf{k}'\in\frac{2\pi}{L}\mathbb{Z}^d,\ |\mathbf{k}-\mathbf{k}'|<\delta} \epsilon_\mu^L(\mathbf{k}')\right)\right). \tag{3.8}$$

Throughout most of our paper, the chemical potential μ is considered to be the natural parameter of our problem. It often can be proven that the energy density exists in the thermodynamic limit for a fixed $\mu \geq 0$

$$e_\mu := \lim_{L\to\infty}\frac{E_\mu^L}{V}. \tag{3.9}$$

and is related to e^ρ of (1.13) by the Legendre transformation

$$e_\mu = \inf_\rho\{e^\rho - \mu\rho\}.$$

By definition, e_μ is decreasing and concave. Hence it is differentiable almost everywhere. At the points of differentiability, we can pass from the grandcanonical to the canonical approach by

$$-\partial_\mu e_\mu = \rho \tag{3.10}$$

At the points where (3.10) has a unique solution $\mu(\rho)$, we should be able to relate the canonical and the grandcanonical IES:

Conjecture 3.2. $\epsilon^\rho(\mathbf{k}) = \epsilon_{\mu(\rho)}(\mathbf{k})$.

The following proposition is one of few rigorous facts that can be easily shown about the IES:

Proposition 3.3. *At zero total momentum, the excitation spectrum has a global minimum where it equals zero: $\epsilon^{L,n}(\mathbf{0}) = \epsilon^{\rho}(\mathbf{0}) = 0$ and $\epsilon_\mu^L(\mathbf{0}) = \epsilon_\mu(\mathbf{0}) = 0$.*

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 (3.1) so does E_μ^L. Hence $\epsilon^{L,n}(\mathbf{0}) = \epsilon_\mu^L(\mathbf{0}) = 0$. □

Let us now formulate the conjectures about $\epsilon_\mu(\mathbf{k})$ (analogous to the Conjecture 1.1 about $\epsilon^\rho(\mathbf{k})$):

Conjecture 3.4. *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 $L \to \infty$, $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$, and $\mathbf{k}_L \to \mathbf{k}$, we have that $\epsilon_\mu^L(\mathbf{k}_L) \to \epsilon_\mu(\mathbf{k})$.
(3) If $d \geq 2$, then $\inf_{\mathbf{k}\neq\mathbf{0}} \frac{\epsilon_\mu(\mathbf{k})}{|\mathbf{k}|} =: c_{\mathrm{cr},\mu} > 0$.
(4) The limit $\lim_{\mathbf{k}\to\mathbf{0}} \frac{\epsilon_\mu(\mathbf{k})}{|\mathbf{k}|} =: c_{\mathrm{ph},\mu} > 0$ exists.
(5) $\mathbf{k} \mapsto \epsilon_\mu(\mathbf{k})$ is subadditive.

3.2. ***c*-number substitution.** One of the steps of the Bogoliubov method consists in replacing the operators $a_{\mathbf{0}}^*$, $a_{\mathbf{0}}$ with c-numbers:

$$a_{\mathbf{0}}^* a_{\mathbf{0}} \approx |\alpha|^2, \quad a_{\mathbf{0}} \approx \alpha, \quad a_{\mathbf{0}}^* \approx \overline{\alpha}. \tag{3.11}$$

This means replacing H_μ^L by

$$\begin{aligned} H_\mu^L(\alpha) \;=\; & \frac{\hat{v}(\mathbf{0})}{2V}|\alpha|^4 - \mu|\alpha|^2 + {\sum_{\mathbf{k}}}' \left(\frac{1}{2}\mathbf{k}^2 - \mu + \frac{\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k})}{V}|\alpha|^2\right) a_{\mathbf{k}}^* a_{\mathbf{k}} \\ & + {\sum_{\mathbf{k}}}' \left(\frac{\hat{v}(\mathbf{k})\alpha^2}{2V} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + \frac{\hat{v}(\mathbf{k})\overline{\alpha}^2}{2V} a_{\mathbf{k}} a_{-\mathbf{k}}\right) \\ & + {\sum_{\mathbf{k}}}' \overline{\alpha} \frac{\hat{v}(\mathbf{k}_1) + \hat{v}(\mathbf{k}_1 + \mathbf{k}_2)}{2V} a_{\mathbf{k}_1+\mathbf{k}_2}^* a_{\mathbf{k}_1} a_{\mathbf{k}_2} \\ & + {\sum_{\mathbf{k}}}' \alpha \frac{\hat{v}(\mathbf{k}_1) + \hat{v}(\mathbf{k}_1 + \mathbf{k}_2)}{2V} a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_1+\mathbf{k}_2} \\ & + \frac{1}{2V} {\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}}' \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\hat{v}(\mathbf{k}_2 - \mathbf{k}_3) a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}. \end{aligned} \tag{3.12}$$

Here ${\sum_{\mathbf{k}}}'$ denotes the sum over all $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d \backslash \{\mathbf{0}\}$. Note that $H_\mu^L(\alpha)$ is the Wick symbol of the operator H_μ^L with respect to the mode $\mathbf{k} = \mathbf{0}$. It is easy to compute also its anti-Wick symbol

$$\tilde{H}_\mu^L(\alpha) = H_\mu^L(\alpha) - \frac{2\hat{v}(\mathbf{0})}{V}|\alpha|^2 + \frac{\hat{v}(\mathbf{0})}{V} + \mu - {\sum_{\mathbf{k}}}' \frac{\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k})}{V} a_{\mathbf{k}}^* a_{\mathbf{k}}.$$

(See e.g. Appendix D for the definitions and basic properties of Wick and anti-Wick symbols).

The following theorem is due to Lieb, Seiringer and Yngvason [22].

Theorem 3.5. *Assume that the energy density e_μ exists. Assume also that $\hat{v}(\mathbf{k})$ is bounded. Then*

$$e_\mu = \lim_{L\to\infty} V^{-1} \inf\{\inf \mathrm{sp} H_\mu^L(\alpha) \;:\; \alpha \in \mathbb{C}\}. \tag{3.13}$$

Thus we can replace H_μ^L with the Hamiltonian $H_\mu^L(\alpha)$ when computing the energy density.

Proof. The anti-Wick symbol of the number operator N^L with respect to the mode $\mathbf{k} = \mathbf{0}$ is

$$\tilde{N}^L(\alpha) = |\alpha|^2 - 1 + \sum_{\mathbf{k}}{}' a_{\mathbf{k}}^* a_{\mathbf{k}}.$$

Note that for $\varphi := \sup_{\mathbf{k}} \hat{v}(\mathbf{k})$, by (D.3) we have

$$0 \leq H_\mu^L(\alpha) - \tilde{H}_\mu^L(\alpha) \leq \frac{2\varphi}{V}\tilde{N}^L + \frac{\hat{v}(\mathbf{0})}{V} - \mu.$$

Now

$$\begin{aligned}
\inf \mathrm{sp} H_\mu^L &\leq \inf\left\{\inf \mathrm{sp} H_\mu^L(\alpha) \ : \ \alpha \in \mathbb{C}\right\} \\
&\leq \inf\left\{\inf \mathrm{sp}\tilde{H}_\mu^L(\alpha) + \frac{2\varphi}{V}\tilde{N}^L(\alpha) \ : \ \alpha \in \mathbb{C}\right\} + \frac{\hat{v}(\mathbf{0})}{V} - \mu \\
&\leq \inf \mathrm{sp} H_{\mu - \frac{2\varphi}{V}}^L + \frac{\hat{v}(\mathbf{0})}{V} - \mu \\
&\leq \inf \mathrm{sp} H_{\mu_1}^L + \frac{\hat{v}(\mathbf{0})}{V} - \mu,
\end{aligned}$$

where in the last inequality $\mu_1 < \mu$ and V is large enough. (The first and third inequality follow from (D.3)). Dividing both sides by V and letting $L \to \infty$ we obtain

$$e_\mu \leq \lim_{L\to\infty} V^{-1} \inf\{\inf \mathrm{sp} H_\mu^L(\alpha) \ : \ \alpha \in \mathbb{C}\} \leq e_{\mu_1}. \tag{3.14}$$

Now $[0, \mu] \ni \mu_1 \mapsto e_{\mu_1}$ is a finite concave function, hence it is continuous, which implies (3.13). □

3.3. **Bogoliubov method.** Let us describe a version of the Bogoliubov approximation adapted to the grand-canonical approach. A similar discussion can be found e.g. in the review of Zagrebnov-Bru [42].

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

For $\alpha \in \mathbb{C}$, we define the displacement or Weyl operator of the mode $\mathbf{k} = \mathbf{0}$:

$$W_\alpha := \mathrm{e}^{-\alpha a_{\mathbf{0}}^* + \overline{\alpha} a_{\mathbf{0}}}, \tag{3.15}$$

and the corresponding coherent vector $\Omega_\alpha := W_\alpha^* \Omega$. Note that W_α is the only Weyl operator commuting with the momentum, and hence Ω_α is the only coherent vector of momentum zero.

Let us apply the "Bogoliubov translation" to the mode $\mathbf{k} = \mathbf{0}$ of H^L. This means making the substitution

$$\begin{aligned}
a_{\mathbf{0}} = \tilde{a}_{\mathbf{0}} + \alpha, &\quad a_{\mathbf{0}}^* = \tilde{a}_{\mathbf{0}}^* + \overline{\alpha}, \\
a_{\mathbf{k}} = \tilde{a}_{\mathbf{k}}, &\quad a_{\mathbf{k}}^* = \tilde{a}_{\mathbf{k}}^*, \qquad \mathbf{k} \neq \mathbf{0}.
\end{aligned} \tag{3.16}$$

Note that

$$\tilde{a}_{\mathbf{k}} = W_\alpha^* a_{\mathbf{k}} W_\alpha, \quad \tilde{a}_{\mathbf{k}}^* = W_\alpha^* a_{\mathbf{k}}^* W_\alpha,$$

and thus the operators with and without tildes satisfy the same commutation relations. In addition, the annihilation operators with tildes kill the "new vacuum" Ω_α.

For notational simplicity, in what follows we drop the tildes and we obtain

$$
\begin{aligned}
H^L &= -\mu|\alpha|^2 + \frac{\hat{v}(\mathbf{0})}{2V}|\alpha|^4 \\
&+ \left(\frac{\hat{v}(\mathbf{0})}{V}|\alpha|^2 - \mu\right)(\overline{\alpha}a_{\mathbf{0}} + \alpha a_{\mathbf{0}}^*) \\
&+ \sum_{\mathbf{k}} \left(\frac{1}{2}\mathbf{k}^2 - \mu + \frac{(\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k}))}{V}|\alpha|^2\right) a_{\mathbf{k}}^* a_{\mathbf{k}} \\
&+ \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{2V}\left(\overline{\alpha}^2 a_{\mathbf{k}} a_{-\mathbf{k}} + \alpha^2 a_{\mathbf{k}}^* a_{-\mathbf{k}}^*\right) \\
&+ \sum_{\mathbf{k},\mathbf{k}'} \frac{\hat{v}(\mathbf{k})}{V}(\overline{\alpha} a_{\mathbf{k}+\mathbf{k}'}^* a_{\mathbf{k}} a_{\mathbf{k}'} + \alpha a_{\mathbf{k}}^* a_{\mathbf{k}'}^* a_{\mathbf{k}+\mathbf{k}'}) \\
&+ \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\frac{\hat{v}(\mathbf{k}_2 - \mathbf{k}_3)}{2V} a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}.
\end{aligned} \tag{3.17}
$$

The expectation value of the state given by Ω_α equals the constant term of (3.17), that is

$$
(\Omega_\alpha | H^L \Omega_\alpha) = -\mu|\alpha|^2 + \frac{\hat{v}(\mathbf{0})}{2V}|\alpha|^4. \tag{3.18}
$$

(3.18) is minimized for $|\alpha|^2 = \mu\frac{V}{\hat{v}(\mathbf{0})}$. This choice kills also the linear term on the second line of (3.17).

Let us choose α so as to minimize (3.18). This means, we choose $\mathrm{e}^{\mathrm{i}\tau}$ and set $\alpha = \mathrm{e}^{\mathrm{i}\tau}\frac{\sqrt{V\mu}}{\sqrt{\hat{v}(\mathbf{0})}}$. Then the Hamiltonian becomes

$$
\begin{aligned}
H^L &:= -V\frac{\mu^2}{2\hat{v}(\mathbf{0})} \\
&+ \sum_{\mathbf{k}} \left(\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})}\right) a_{\mathbf{k}}^* a_{\mathbf{k}} \\
&+ \sum_{\mathbf{k}} \hat{v}(\mathbf{k})\frac{\mu}{2\hat{v}(\mathbf{0})}\left(\mathrm{e}^{-\mathrm{i}2\tau}\, a_{\mathbf{k}} a_{-\mathbf{k}} + \mathrm{e}^{\mathrm{i}2\tau}\, a_{\mathbf{k}}^* a_{-\mathbf{k}}^*\right) \\
&+ \sum_{\mathbf{k},\mathbf{k}'} \frac{\hat{v}(\mathbf{k})\sqrt{\mu}}{\sqrt{\hat{v}(\mathbf{0})V}}(\overline{\mathrm{e}}^{\mathrm{i}\tau}\, a_{\mathbf{k}+\mathbf{k}'}^* a_{\mathbf{k}} a_{\mathbf{k}'} + \mathrm{e}^{\mathrm{i}\tau}\, a_{\mathbf{k}}^* a_{\mathbf{k}'}^* a_{\mathbf{k}+\mathbf{k}'}) \\
&+ \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\frac{\hat{v}(\mathbf{k}_2 - \mathbf{k}_3)}{2V} a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}.
\end{aligned} \tag{3.19}
$$

(Note that we have made no approximation yet). The first 3 lines of (3.19) form a quadratic Hamiltonian, which will be denoted by H_{bg}^L. Now let us make the assumption that H_{bg}^L can be treated as an approximation to H^L. For a possible justification for this approximation see Subsection 4.1.

It is easy to find the excitation spectrum of H_{bg}^L. To this end, for $\mathbf{k} \neq \mathbf{0}$ we make the substitution

$$
a_{\mathbf{k}}^* = c_{\mathbf{k}} b_{\mathbf{k}}^* - \overline{s}_{\mathbf{k}} b_{-\mathbf{k}}, \quad a_{\mathbf{k}} = c_{\mathbf{k}} b_{\mathbf{k}} - s_{\mathbf{k}} b_{-\mathbf{k}}^*, \tag{3.20}
$$

Let $\theta = (\theta_{\mathbf{k}})$ be a sequence such that $\theta_{\mathbf{0}} = 0$ and

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

Introduce the unitary operator

$$U_\theta := \prod_{\mathbf{k}} \mathrm{e}^{-\frac{1}{2}\theta_{\mathbf{k}} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + \frac{1}{2}\overline{\theta}_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}}. \tag{3.21}$$

Note that

$$U_\theta^* a_{\mathbf{k}} U_\theta = b_{\mathbf{k}}, \qquad U_\theta^* a_{\mathbf{k}}^* U_\theta = b_{\mathbf{k}}^*,$$

and hence $a_{\mathbf{k}}, a_{\mathbf{k}}^*$ satisfy the same commutation relations as $b_{\mathbf{k}}, b_{\mathbf{k}}^*$. Note also that 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 mode $\mathbf{k} = \mathbf{0}$ has to be treated separately. Let us introduce the operators $p_{\mathbf{0}}$ and $x_{\mathbf{0}}$ which are defined as

$$p_{\mathbf{0}} = \frac{1}{\sqrt{2}}(\mathrm{e}^{\mathrm{i}\tau}\, a_{\mathbf{0}}^* + \mathrm{e}^{-\mathrm{i}\tau}\, a_{\mathbf{0}}), \qquad x_{\mathbf{0}} = \frac{\mathrm{i}}{\sqrt{2}}(-\,\mathrm{e}^{\mathrm{i}\tau}\, a_{\mathbf{0}}^* + \mathrm{e}^{-\mathrm{i}\tau}\, a_{\mathbf{0}}). \tag{3.22}$$

They are self-adjoint operators and satisfy the commutation relation $[x_{\mathbf{0}}, p_{\mathbf{0}}] = \mathrm{i}$. As we can see they are the "momentum" and "position" of the mode $\mathbf{k} = \mathbf{0}$.

We choose the Bogoliubov rotation that kills double creators and annihilators, which amounts to

$$s_{\mathbf{k}} \quad = \quad \frac{\alpha}{\sqrt{2}|\alpha|}\left(\left(1 - \left(\frac{\hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})}}{\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})}}\right)^2\right)^{-1/2} - 1\right)^{1/2}. \tag{3.23}$$

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

$$H_{\mathrm{bg}}^L \quad = \quad E_{\mathrm{bg}}^L + \mu p_{\mathbf{0}}^2 + \sum_{\mathbf{k}}{}' \omega_{\mathrm{bg}}(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}}, \tag{3.24}$$

where the elementary excitation spectrum is

$$\omega_{\mathrm{bg}}(\mathbf{k}) = \sqrt{\frac{1}{2}\mathbf{k}^2(\frac{1}{2}\mathbf{k}^2 + 2\hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})})}. \tag{3.25}$$

and the energy is

$$E_{\mathrm{bg}}^L \quad = \quad -V\frac{\mu^2}{2\hat{v}(\mathbf{0})} - \sum_{\mathbf{k}} \frac{1}{2}\left((\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})}) - \omega_{\mathrm{bg}}(\mathbf{k}) \right), \tag{3.26}$$

(where the sum above includes the mode $\mathbf{k} = \mathbf{0}$ again).

Note that $\omega_{\mathrm{bg}}(\mathbf{k})$ is well defined for all values $\mathbf{k} \in \mathbb{R}^d$, even though it is restricted to $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ in (3.24) and (3.26). The IES of H_{bg}^L for $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ is given by

$$\epsilon_{\mathrm{bg}}^L(\mathbf{k}) = \inf\{\omega_{\mathrm{bg}}(\mathbf{k}_1) + \cdots + \omega_{\mathrm{bg}}(\mathbf{k}_n) \ : \ \mathbf{k}_1 + \cdots + \mathbf{k}_n = \mathbf{k}, \ \ \mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d, \ n = 1, 2, \dots\}.$$

The thermodynamic limit of $\epsilon_{\mathrm{bg}}^L(\mathbf{k})$ is defined for any $\mathbf{k} \in \mathbb{R}^d$ by

$$\epsilon_{\mathrm{bg}}(\mathbf{k}) = \inf\{\omega_{\mathrm{bg}}(\mathbf{k}_1) + \cdots + \omega_{\mathrm{bg}}(\mathbf{k}_n) \ : \ \mathbf{k}_1 + \cdots + \mathbf{k}_n = \mathbf{k}, \ \ \mathbf{k} \in \mathbb{R}^d, \ \ n = 1, 2, \dots\}. \tag{3.27}$$

We have (in any dimension)

(1) $\inf_{\mathbf{k} \neq \mathbf{0}} \frac{\omega_{\mathrm{bg}}(\mathbf{k})}{|\mathbf{k}|} = \inf \sqrt{\frac{1}{2}(\frac{1}{2}\mathbf{k}^2 + 2\frac{\hat{v}(\mathbf{k})\mu}{\hat{v}(\mathbf{0})})} =: c_{\mathrm{cr,bg}} > 0$;

(2) $\lim_{\mathbf{k} \to \mathbf{0}} \frac{\omega_{\mathrm{bg}}(\mathbf{k})}{|\mathbf{k}|} = \sqrt{\mu} =: c_{\mathrm{ph,bg}} > 0$.

Therefore, by Theorem A.4 (1) and (2) we have

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

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

Thus, $\epsilon_{\rm bg}(\mathbf{k})$ has all the properties described in Conjecture 3.4.

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

$$s_{\mathbf{k}} \approx \frac{\mathrm{e}^{\mathrm{i}\tau}}{\sqrt{2}}\mu^{1/4}|\mathbf{k}|^{-1/2}. \tag{3.28}$$

(3.24) has no ground state because of the mode $\mathbf{k} = \mathbf{0}$. Let Ψ be any vector that minimizes modes $\mathbf{k} \neq \mathbf{0}$. Clearly, for $\mathbf{k} \neq \mathbf{0}$,

$$(\Psi|a_{\mathbf{k}}^* a_{\mathbf{k}}\Psi) = |s_{\mathbf{k}}|^2 \approx \frac{\mu^{1/2}}{2|\mathbf{k}|}.$$

Let

$$N' := \sum_{\mathbf{k}}{}' a_{\mathbf{k}}^* a_{\mathbf{k}}$$

be the number of particles away from the mode $\mathbf{k} = \mathbf{0}$. Clearly the density of particles away from the mode $\mathbf{k} = \mathbf{0}$ in the state Ψ equals

$$\frac{1}{V}(\Psi|N'\Psi) = \frac{1}{V}\sum_{\mathbf{k}}{}'|s_{\mathbf{k}}|^2. \tag{3.29}$$

We expect that for large L, (3.29) converges to

$$\frac{1}{(2\pi)^d}\int |s_{\mathbf{k}}|^2 \mathrm{d}\mathbf{k}. \tag{3.30}$$

Note that in dimension $d = 1$ there is a problem with the formula (3.30), since $|\mathbf{k}|^{-1}$ is integrable only in dimension $d > 1$. Therefore, for $d = 1$ (3.30) diverges. Thus, the Bogoliubov approximation is problematic for $d = 1$ if we keep the density of particles ρ fixed as $L \to \infty$. To our knowledge, (3.28) and the above described problem of the Bogoliubov approximation in $d = 1$ was first noticed in [9].

Nevertheless, in spite of the breakdown of the Bogoliubov approximation, many authors believe that also in $d = 1$ the IES exhibits the behavior $\epsilon_\mu(\mathbf{k}) \approx c_{\rm ph}|\mathbf{k}|$ with $c_{\rm ph} > 0$ for low momenta, see e.g. [28], Chapter 6, [20, 19].

3.4. **Improving the Bogoliubov method.** For $\frac{2\pi}{L}\mathbb{Z}^d \ni \mathbf{k} \mapsto \theta_{\mathbf{k}} \in \mathbb{C}$, a square summable sequence with $\theta_{\mathbf{k}} = \theta_{-\mathbf{k}}$, let U_θ be defined as in (3.21). (This time we allow $\theta_{\mathbf{0}}$ to be nonzero). For $\alpha \in \mathbb{C}$, let W_α be defined as in (3.15).

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

$$\Omega_{\alpha,\theta} := U_{\alpha,\theta}^*\Omega$$

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

One of our next objectives is to look for the squeezed vector that minimizes the expectation value of H^L. As in Section 3.3, we will also compute the Hamiltonian H^L expressed in new creation and annihilation operators adapted to the new vacuum $\Omega_{\alpha,\theta}$. We do this in two steps. First we perform the Bogoliubov translation (3.16), which results in the expression (3.17). Then we perform the Bogoliubov rotation (3.20). This time, however, we apply it to all the modes, including $\mathbf{k} = \mathbf{0}$.

The Hamiltonian after these substitutions in the Wick ordered form equals

$$\begin{aligned} H^L = {} & B^L + C^L b_{\mathbf{0}}^* + \overline{C}^L b_{\mathbf{0}} \\ & + \frac{1}{2}\sum_{\mathbf{k}} O^L(\mathbf{k}) b_{\mathbf{k}}^* b_{-\mathbf{k}}^* + \frac{1}{2}\sum_{\mathbf{k}} \overline{O}^L(\mathbf{k}) b_{\mathbf{k}} b_{-\mathbf{k}} + \sum_{\mathbf{k}} D^L(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}} \\ & + \text{terms higher order in } b\text{'s}. \end{aligned} \tag{3.31}$$

Clearly,

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

Therefore, we obtain rigorous bounds

$$E^L \leq B^L, \quad E^L + \epsilon^L(\mathbf{k}) \leq B^L + D^L(\mathbf{k}).$$

If we require that B^L attains its minimum, then we will later on show that C^L and $O^L(\mathbf{k})$ vanish for all $\mathbf{k}$. Henceforth we drop the superscript L.

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

In order to express $D(\mathbf{k})$ and $O(\mathbf{k})$, it is convenient to introduce

$$f_{\mathbf{k}} := \frac{\mathbf{k}^2}{2} - \mu + |\alpha|^2 \frac{\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k})}{V} + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k}) + \hat{v}(\mathbf{0})}{V} |s_{\mathbf{k}'}|^2, \tag{3.32}$$

$$g_{\mathbf{k}} := \alpha^2 \frac{\hat{v}(\mathbf{k})}{V} - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{V} s_{\mathbf{k}'} c_{\mathbf{k}'}. \tag{3.33}$$

(Note that $f_{\mathbf{k}}$ is real).

$$D(\mathbf{k}) = f_{\mathbf{k}}(c_{\mathbf{k}}^2 + |s_{\mathbf{k}}|^2) - c_{\mathbf{k}}(s_{\mathbf{k}} \overline{g}_{\mathbf{k}} + \overline{s}_{\mathbf{k}} g_{\mathbf{k}}), \tag{3.34}$$

$$O(\mathbf{k}) = -2 c_{\mathbf{k}} s_{\mathbf{k}} f_{\mathbf{k}} + s_{\mathbf{k}}^2 \overline{g}_{\mathbf{k}} + c_{\mathbf{k}}^2 g_{\mathbf{k}}. \tag{3.35}$$

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

3.5. **Conditions arising from minimization of the energy over α.** We demand that B attains a minimum. To this end we first compute the derivatives with respect to α and $\overline{\alpha}$:

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

Note that

$$C = c_{\mathbf{0}} \partial_{\overline{\alpha}} B - s_{\mathbf{0}} \partial_\alpha B,$$

so that the condition

$$\partial_{\overline{\alpha}} B = \partial_\alpha B = 0 \tag{3.36}$$

entails $C = 0$. The condition (3.36) yields

$$\mu = \frac{\hat{v}(\mathbf{0})}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k}')}{V}|s_{\mathbf{k}'}|^2 - \frac{\alpha^2}{|\alpha|^2} \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{V}\overline{s}_{\mathbf{k}'} c_{\mathbf{k}'}. \tag{3.37}$$

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

$$f_{\mathbf{k}} := \frac{\mathbf{k}^2}{2} + |\alpha|^2 \frac{\hat{v}(\mathbf{k})}{V} + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}' - \mathbf{k}) - \hat{v}(\mathbf{k}')}{V}|s_{\mathbf{k}'}|^2 + \frac{\alpha^2}{|\alpha|^2} \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{V}\overline{s}_{\mathbf{k}'} c_{\mathbf{k}'}. \tag{3.38}$$

3.6. **Conditions arising from minimization of the energy over $s_{\mathbf{k}}$.** Computing the derivative with respect to $s_{\mathbf{k}}$, $\overline{s}_{\mathbf{k}}$ we can use

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

$$\partial_{s_{\mathbf{k}}} B = f_{\mathbf{k}}\overline{s}_{\mathbf{k}} - \frac{\overline{g}_{\mathbf{k}}}{2}\left(c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{2c_{\mathbf{k}}}\right) - g_{\mathbf{k}}\frac{\overline{s}_{\mathbf{k}}^2}{4c_{\mathbf{k}}}, \tag{3.39}$$

$$\partial_{\overline{s}_{\mathbf{k}}} B = f_{\mathbf{k}} s_{\mathbf{k}} - \frac{g_{\mathbf{k}}}{2}\left(c_{\mathbf{k}} + \frac{|s_{\mathbf{k}}|^2}{2c_{\mathbf{k}}}\right) - \overline{g}_{\mathbf{k}}\frac{s_{\mathbf{k}}^2}{4c_{\mathbf{k}}}. \tag{3.40}$$

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 $O(\mathbf{k}) = 0$.

(3.39) and (3.40) also imply

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

and hence

$$g_{\mathbf{k}}\overline{s}_{\mathbf{k}} = \overline{g}_{\mathbf{k}} s_{\mathbf{k}}. \tag{3.41}$$

It is convenient to introduce the parameters

$$S_{\mathbf{k}} := 2 s_{\mathbf{k}} c_{\mathbf{k}},$$
$$C_{\mathbf{k}} := c_{\mathbf{k}}^2 + |s_{\mathbf{k}}|^2.$$

Now, using (3.41) we can write

$$D(\mathbf{k}) = C_{\mathbf{k}} f_{\mathbf{k}} - S_{\mathbf{k}}\overline{g}_{\mathbf{k}}, \tag{3.42}$$

$$O(\mathbf{k}) = -S_{\mathbf{k}} f_{\mathbf{k}} + C_{\mathbf{k}} g_{\mathbf{k}}. \tag{3.43}$$

Equating $O(\mathbf{k})$ to zero and assuming that $f_{\mathbf{k}} \neq \mathbf{0}$ we obtain

$$D(\mathbf{k}) = \mathrm{sgn} f_{\mathbf{k}} \sqrt{f_{\mathbf{k}}^2 - |g_{\mathbf{k}}|^2}, \tag{3.44}$$

$$S_{\mathbf{k}} = \frac{g_{\mathbf{k}}}{D(\mathbf{k})}, \tag{3.45}$$

$$C_{\mathbf{k}} = \frac{f_{\mathbf{k}}}{D(\mathbf{k})}. \tag{3.46}$$

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. We set $\mathrm{e}^{\mathrm{i}\tau} := \frac{\alpha}{|\alpha|}$. Then we can write

$$\begin{aligned} f_{\mathbf{k}} : &= \frac{\mathbf{k}^2}{2} + |\alpha|^2 \frac{\hat{v}(\mathbf{k})}{V} \\ &+ \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k}) - \hat{v}(\mathbf{k}')}{2V}(C_{\mathbf{k}'} - 1) + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{2V} \mathrm{e}^{\mathrm{i}2\tau} \overline{S}_{\mathbf{k}'}, \qquad (3.47) \\ g_{\mathbf{k}} : &= \alpha^2 \frac{\hat{v}(\mathbf{k})}{V} - \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}'-\mathbf{k})}{2V} S_{\mathbf{k}'}. \qquad (3.48) \end{aligned}$$

Then we can express μ by

$$\mu = \frac{\hat{v}(\mathbf{0})}{V}|\alpha|^2 + \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k}')}{2V}(C_{\mathbf{k}'} - 1) - \mathrm{e}^{\mathrm{i}2\tau} \sum_{\mathbf{k}'} \frac{\hat{v}(\mathbf{k}')}{2V} \overline{S}_{\mathbf{k}'}. \qquad (3.49)$$

One can express the minimizing conditions in the following theorem.

Theorem 3.6. *(1) Suppose that $|\alpha|^2 > 0$ and $\mathrm{e}^{\mathrm{i}\tau}$ are fixed parameters. Let the first derivative of B with respect to $\alpha, \overline{\alpha}, (s_{\mathbf{k}}), (\overline{s}_{\mathbf{k}})$ vanish. Let $f_{\mathbf{k}}$, $g_{\mathbf{k}}$ be given by (3.47), (3.48). For any $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$ we have then $f_{\mathbf{k}}^2 \geq |g_{\mathbf{k}}|^2$, and the equations (3.44)–(3.46) hold.*

(2) We have

$$\begin{bmatrix} \partial_{\overline{\alpha}}\partial_{\alpha} B & \partial_{\overline{\alpha}}^2 B \\ \partial_{\alpha}^2 B & \partial_{\alpha}\partial_{\overline{\alpha}} B \end{bmatrix} = \begin{bmatrix} f_0 & g_0 \\ \overline{g}_0 & f_0 \end{bmatrix}. \qquad (3.50)$$

(3.50) is positive/negative definite iff $D(\mathbf{0})$ is positive/negative. (3.50) is zero iff $D(\mathbf{0}) = 0$. Besides,

$$D(\mathbf{0}) = 2\mathrm{sgn} f_0 \sqrt{\frac{\hat{v}(\mathbf{0})}{V} \alpha^2 \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k})}{2V} \overline{S}_{\mathbf{k}}} \qquad (3.51)$$

In the above theorem we included all possibilities that guarantee the stationarity of B. Clearly, the case of $D(\mathbf{k}) < 0$ seems physically irrelevant. But this is equivalent to $f_{\mathbf{k}} < 0$. Therefore, under the additional condition $D(\mathbf{k}) \geq 0$, we can drop $\mathrm{sgn} f_{\mathbf{k}}$ from (3.44).

In the case of the zero momentum we have an additional argument for the positivity of $D(\mathbf{0})$ given in (2). $D(\mathbf{0}) \geq 0$ is in fact equivalent to the condition (3.50)≥ 0, which is necessary for the existence of minimum of B.

Let us compute the ground state energy in the improved Bogoliubov method. Inserting (3.37) to the expression for B we obtain

$$\begin{aligned} B &= -\frac{\hat{v}(\mathbf{0})}{2V}\left(|\alpha|^2 + \sum_{\mathbf{k}} |s_{\mathbf{k}}|^2\right)^2 + \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2}|s_{\mathbf{k}}|^2 \\ &+ \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k}-\mathbf{k}') - \hat{v}(\mathbf{k}') - v(\mathbf{k})}{2V} |s_{\mathbf{k}'}|^2 |s_{\mathbf{k}}|^2 \\ &+ \sum_{\mathbf{k}} \frac{\hat{v}(\mathbf{k}')}{4V}(\mathrm{e}^{\mathrm{i}2\tau} \overline{S}_{\mathbf{k}} + \mathrm{e}^{-\mathrm{i}2\tau} S_{\mathbf{k}})|s_{\mathbf{k}}|^2 \\ &+ \sum_{\mathbf{k},\mathbf{k}'} \frac{\hat{v}(\mathbf{k}-\mathbf{k}')}{8V} S_{\mathbf{k}'} \overline{S}_{\mathbf{k}}, \end{aligned}$$

where recall that $|s_{\mathbf{k}}|^2 = \frac{1}{2}(C_{\mathbf{k}} - 1)$. Using (3.37) 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

$$\rho = \frac{|\alpha|^2 + \sum_{\mathbf{k}} |s_{\mathbf{k}}|^2}{V}. \tag{3.52}$$

3.7. **Thermodynamic limit of the fixed point equation.** One can ask whether the method described in the previous two sections has a well defined limit as $L \to \infty$. A natural way to take this limit, at least formally, involves the following steps. We put $\alpha = \sqrt{V\kappa}\,\mathrm{e}^{\mathrm{i}\tau}$, for some fixed parameter $\kappa > 0$ having the interpretation of the density of the condensate. We expect $s_{\mathbf{k}}$ (and hence $S_{\mathbf{k}}$, etc.) to converge to a function depending on $\mathbf{k} \in \mathbb{R}^d$ in a reasonable class. Finally, we replace $\frac{1}{V}\sum\limits_{\mathbf{k}}$ by $\frac{1}{(2\pi)^d}\int \mathrm{d}\mathbf{k}$. Thus equations (3.47), (3.48) and (3.49) are replaced with

$$\begin{aligned}
f_{\mathbf{k}} &= \frac{\mathbf{k}^2}{2} + \kappa\hat{v}(\mathbf{k}) + \frac{1}{2(2\pi)^d}\int (\hat{v}(\mathbf{k}'-\mathbf{k}) - \hat{v}(\mathbf{k}'))(C_{\mathbf{k}'} - 1)\mathrm{d}\mathbf{k}' \\
&\quad + \frac{\mathrm{e}^{\mathrm{i}2\tau}}{2(2\pi)^d}\int \hat{v}(\mathbf{k}')\overline{S}_{\mathbf{k}'}\mathrm{d}\mathbf{k}', && (3.53)\\
g_{\mathbf{k}} &= \kappa\,\mathrm{e}^{\mathrm{i}2\tau}\,\hat{v}(\mathbf{k}) - \frac{1}{2(2\pi)^d}\int \hat{v}(\mathbf{k}'-\mathbf{k})S_{\mathbf{k}'}\mathrm{d}\mathbf{k}', && (3.54)\\
\mu &= \hat{v}(\mathbf{0})\kappa + \frac{1}{2(2\pi)^d}\int (\hat{v}(\mathbf{0}) + \hat{v}(\mathbf{k}'))(C_{\mathbf{k}'} - 1)\mathrm{d}\mathbf{k}' \\
&\quad - \frac{\mathrm{e}^{\mathrm{i}2\tau}}{2(2\pi)^d}\int \hat{v}(\mathbf{k}')\overline{S}_{\mathbf{k}'}\mathrm{d}\mathbf{k}'. && (3.55)
\end{aligned}$$

We also obtain (in the physical case of positive D)

$$D(\mathbf{0}) = 2\sqrt{\hat{v}(\mathbf{0})\kappa\frac{1}{2(2\pi)^d}\int \mathrm{d}\mathbf{k}\hat{v}(\mathbf{k})\overline{S}_{\mathbf{k}}}. \tag{3.56}$$

(3.56) is typically positive – thus the quadratic part of the Hamiltonian (3.31) seems to have a gap.

One can try to find $\alpha, (S_{\mathbf{k}})$ satisfying the minimization condition by iterations. A natural starting point seems to be $S_{\mathbf{k}} = 0$. Then, by (3.37) or (3.55), $\mu = \hat{v}(\mathbf{0})\kappa$. After one iteration we obtain

$$\begin{aligned}
f_{\mathbf{k}} &= \frac{\mathbf{k}^2}{2} + \kappa\hat{v}(\mathbf{k}),\\
g_{\mathbf{k}} &= \kappa\hat{v}(\mathbf{k}),\\
D(\mathbf{k}) &= \sqrt{(\mathbf{k}^2/2)^2 + \mathbf{k}^2\kappa\hat{v}(\mathbf{k})},\\
S_{\mathbf{k}} &= \frac{\kappa\hat{v}(\mathbf{k})}{\sqrt{(\mathbf{k}^2/2)^2 + \mathbf{k}^2\kappa\hat{v}(\mathbf{k})}}
\end{aligned}$$

Thus $D(\mathbf{k}) = \omega_{\mathrm{bg},\mu}(\mathbf{k})$ given by (3.25) – we obtain the grand-canonical Bogoliubov approximation.

In the case of finite L we cannot continue iterations because of $S_0 = \infty$.

In the thermodynamic limit, the value at zero may not matter, since $\mathbf{k}$ is a continuous variable. $S_{\mathbf{k}}$ for small $\mathbf{k}$ behaves as $\sim |\mathbf{k}|^{-1}$ (this was noted already in (3.23)). In dimension $d = 1$, if we try to do the next iteration we obtain divergent integrals. Thus, we cannot continue iterations. However in dimensions $d \geq 2$ the integrals are convergent and we can do the next iteration (and presumably we can keep on going).

The energy gap appears already at the second iteration.

3.8. **Uncorrelated states.** Let $\mathcal{H}_0$ denote the space spanned by 1 and let $\mathcal{H}_{\{\mathbf{k},-\mathbf{k}\}}$ denote the space spanned by $\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}}$ and $\mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{x}}$. Clearly,

$$L^2(\Lambda) = \mathcal{H}_0 \oplus \left(\underset{\{\mathbf{k},-\mathbf{k}\}}{\oplus} \mathcal{H}_{\{\mathbf{k},-\mathbf{k}\}} \right). \tag{3.57}$$

The sum in (3.57) runs over all two-element sets of the form $\{\mathbf{k}, -\mathbf{k}\}$ with $\mathbf{k} \in \frac{2\pi}{L}\mathbb{Z}^d$.

The exponential property of Fock spaces yields

$$\Gamma_{\mathrm{s}}(L^2(\Lambda)) = \Gamma_{\mathrm{s}}(\mathcal{H}_0) \otimes \left(\underset{\{\mathbf{k},-\mathbf{k}\}}{\otimes} \Gamma_{\mathrm{s}}(\mathcal{H}_{\{\mathbf{k},-\mathbf{k}\}}) \right). \tag{3.58}$$

(See e.g. [37] for the definition of the tensor product of an infinite family of Hilbert spaces used in (3.58). Note that in each of the factors of the tensor product of (3.58) we distinguish a normalized vector – the vacuum vector).

We will say that a vector $\Psi \in \Gamma_{\mathrm{s}}(L^2(\Lambda))$ is uncorrelated with respect to (3.58), or simply *uncorrelated*, iff it is of the form

$$\Psi = \Psi_0 \otimes \left(\underset{\{\mathbf{k},-\mathbf{k}\}}{\otimes} \Psi_{\{\mathbf{k},-\mathbf{k}\}}) \right)$$

for some

$$\Psi_0 \in \Gamma_{\mathrm{s}}(\mathcal{H}_0), \quad \Psi_{\{\mathbf{k},-\mathbf{k}\}} \in \Gamma_{\mathrm{s}}(\mathcal{H}_{\{\mathbf{k},-\mathbf{k}\}}).$$

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

$$E^L_{\mathrm{un}} := \inf \left\{ (\Psi|H^L\Psi) \ : \ \Psi \text{ is uncorrelated and of norm } 1 \right\}.$$

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

$$\epsilon^L_{\mathrm{un}}(\mathbf{k}) := \inf \left\{ (\Psi|H^L(\mathbf{k})\Psi) - E^L_{\mathrm{un}} \ : \ \Psi \text{ is uncorrelated, } \|\Psi\| = 1 \right\},$$

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

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

Clearly, from the mini-max principle we obtain

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

Conjecture 3.7. *We believe the following statements to hold true:*

(1) The map $\mathbb{R}^d \ni \mathbf{k} \mapsto \epsilon_{\mathrm{un}}(\mathbf{k}) \in \mathbb{R}$ is positive and continuous away from 0.

(2) Let $\mathbf{k} \in \mathbb{R}^d\backslash\{0\}$. If $L \to \infty$, $\mathbf{k}_L \in \frac{2\pi}{L}\mathbb{Z}^d$, and $\mathbf{k}_L \to \mathbf{k}$, then $\epsilon^L_{\mathrm{un}}(\mathbf{k}_L) \to \epsilon_{\mathrm{un}}(\mathbf{k})$.

(3) $\sup_{\mathbf{k}\neq\mathbf{0}} \epsilon_{\mathrm{un}}(\mathbf{k}) > 0$.

Thus we conjecture that using only uncorrelated states in a variational determination of the excitation spectrum have serious limitations. We expect the results to be well behaved in the thermodynamic limit, but they will probably not capture the phononic behavior at the bottom of the IES, and in particular we will obtain an energy gap.

Note that the squeezed vectors $\Omega_{\alpha,\theta}$ and the particle excitations over the squeezed vectors $b^*_{\mathbf{k}}\Omega_{\alpha,\theta}$ are examples of uncorrelated vectors. Therefore, the expectation values of H^L in these vectors give an upper bound on E^L_{un} and $E^L_{\mathrm{un}} + \epsilon^L_{\mathrm{un}}(\mathbf{k})$. We showed that for these expectation values one should expect an energy gap – we expect this gap to persist even for more general uncorrelated states.

Thus, in order to obtain more satisfactory bounds it seems that one needs to use *correlated* vectors. Note that the Bijls-Feynman variational vector $N_{\mathbf{k}}\Psi/\|N_{\mathbf{k}}\Psi\|$ is correlated for $\mathbf{k} \neq \mathbf{0}$, even if Ψ is uncorrelated.

4. Perturbative approach

In this section we will use the grand-canonical formalism. We replace the potential $v(\mathbf{x})$ with $\lambda v(\mathbf{x})$, where λ is a (small) positive constant. We will drop μ from most symbols and instead we will make the dependence on λ explicit. Thus instead H_μ^L we will write $H^{\lambda,L}$.

4.1. **Perturbative approach based on the Bogoliubov method.** Let us go back to the Bogoliubov method described in Subsection 3.3. Using the formula (3.19) we can split the Hamiltonian as

$$H^{\lambda,L} = \lambda^{-1} H_{-1}^L + H_0^L + \sqrt{\lambda} H_{\frac{1}{2}}^L + \lambda H_1^L,$$

where

$$\begin{aligned}
H_{-1}^L &:= -V\frac{\mu^2}{2\hat{v}(\mathbf{0})}, \qquad (4.1)\\
H_0^L &:= \sum_{\mathbf{k}} \left(\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})}\right) a_{\mathbf{k}}^* a_{\mathbf{k}} \\
&+ \sum_{\mathbf{k}} \hat{v}(\mathbf{k}) \frac{\mu}{2\hat{v}(\mathbf{0})} \left(\mathrm{e}^{-\mathrm{i}2\tau}\, a_{\mathbf{k}} a_{-\mathbf{k}} + \mathrm{e}^{\mathrm{i}2\tau}\, a_{\mathbf{k}}^* a_{-\mathbf{k}}^*\right),\\
H_{\frac{1}{2}}^L &:= \sum_{\mathbf{k},\mathbf{k}'} \frac{\hat{v}(\mathbf{k})\sqrt{\mu}}{\sqrt{\hat{v}(\mathbf{0})V}} (\overline{\mathrm{e}}^{\mathrm{i}\tau} a_{\mathbf{k}+\mathbf{k}'}^* a_{\mathbf{k}} a_{\mathbf{k}'} + \mathrm{e}^{\mathrm{i}\tau}\, a_{\mathbf{k}}^* a_{\mathbf{k}'}^* a_{\mathbf{k}+\mathbf{k}'}),\\
H_1^L &:= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4) \frac{\hat{v}(\mathbf{k}_2-\mathbf{k}_3)}{2V} a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}.
\end{aligned}$$

Note that H_n^L, $n = -1, 0, \frac{1}{2}, 1$, do not depend on λ. This suggests that one can try to apply methods of perturbation theory to compute the ground state energy of $H^{\lambda,L}$ treating $\sqrt{\lambda}H_{\frac{1}{2}} + \lambda H_1$ as a small perturbation of the quadratic Bogoliubov Hamiltonian

$$\lambda^{-1} H_{-1}^L + H_0^L. \qquad (4.2)$$

It is also tempting to compute the excitation spectrum, applying perturbation methods to the same splitting of $H^{\lambda,L}$ restricted to the sector of fixed momentum $\mathbf{k}$. Unfortunately, when one tries to implement this idea one encounters serious difficulties due to the infrared problem: the operator (4.2) does not have a ground state, neither globally, nor in fixed momentum sectors (because of the $\mathbf{k} = \mathbf{0}$ mode). Further on we will describe a natural approach that should help solve the infrared problem and should give a better starting point for the perturbation methods.

In any case, the splitting suggests the following conjecture (which is the grand-canonical version of Conjecture 1.2). Let $\epsilon_\mu^\lambda(\mathbf{k})$ be the grand-canonical IES for the potential λv and let $\epsilon_{\mathrm{bg},\mu}(\mathbf{k})$ be given by (3.27).

Conjecture 4.1. *Let $d \geq 2$. Then for a large class of repulsive potentials we have*

$$\lim_{\lambda \searrow 0} \epsilon_\mu^\lambda(\mathbf{k}) = \epsilon_{\mathrm{bg},\mu}(\mathbf{k}).$$

4.2. **Perturbative approach based on improved Bogoliubov method.** We fix the size of the box, μ and $\mathrm{e}^{\mathrm{i}\tau}$ and we assume that we solved the fixed point equation described in Subsection 3.6 and there is an energy gap. We assume that the solution is unique. The expression for $H^{\lambda,L}$ Wick-ordered with respect to the operators $b_{\mathbf{k}}$, $b_{\mathbf{k}}^*$ allows us to write

$$H^{\lambda,L} = \lambda^{-1} H_{-1}^{\lambda,L} + H_0^{\lambda,L} + \sqrt{\lambda} H_{\frac{1}{2}}^{\lambda,L} + \lambda H_1^{\lambda,L}, \tag{4.3}$$

where $\lambda^{-1}H_{-1}^{\lambda,L} = B$ is the constant term, $H_1^{\lambda,L} = \sum_{\mathbf{k}} D(\mathbf{k}) b_{\mathbf{k}}^* b_{\mathbf{k}}$ is the quadratic term, $H_{\frac{1}{2}}^{\lambda,L}$ and $H_1^{\lambda,L}$ are respectively the third and fourth order parts of H in operators $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^*$, see (3.31).

The splitting (4.3) can be used to set up a perturbatve approach for computing the energy density and excitation spectrum. The presence of a gap will be actually an advantage in this case.

More precisely, let us consider the following Hamiltonian

$$H^{\lambda,\delta,L} := \delta^{-1} H_{-1}^{\lambda,L} + H_0^{\lambda,L} + \sqrt{\delta} H_{\frac{1}{2}}^{\lambda,L} + \delta H_1^{\lambda,L}, \tag{4.4}$$

where δ is an additional parameter introduced for bookkeeping reasons. We treat $\delta^{-1}H_{-1}^{\lambda,L} + H_0^{\lambda,L}$ as the unperturbed operator and the rest as a perturbation depending on the small parameter δ. $\delta^{-1}H_{-1}^{\lambda,L} + H_0^{\lambda,L}$ has a ground state $\Omega_{\alpha,\theta}$, and even a mass gap, so the perturbation expansion in terms of δ for the ground state vector and energy is well defined and for small δ

$$\Psi^{\lambda,\delta,L} = \sum_{n=0}^{\infty} (\delta^n \Psi_n^{\lambda,L} + \delta^{n+\frac{1}{2}} \Psi_{n+\frac{1}{2}}^{\lambda,L}), \quad E^{\lambda,\delta,L} = \sum_{n=-1}^{\infty} \delta^n E_n^{\lambda,L},$$

where $\Psi_0^{\lambda,L} = \Omega_{\alpha,\theta}$. (It is easy to see that all powers of δ for the energy are integral). At the end we will substitute λ for δ:

$$\Psi^{\lambda,L} \sim \sum_{n=0}^{\infty} (\lambda^n \Psi_n^{\lambda,L} + \lambda^{n+\frac{1}{2}} \Psi_{n+\frac{1}{2}}^{\lambda,L}), \quad E^{\lambda,L} \sim \sum_{n=-1}^{\infty} \lambda^n E_n^{\lambda,L}. \tag{4.5}$$

Let $\epsilon^L(\mathbf{k})$ be the subadditive hull of $D^L(\mathbf{k})$. Assume that for some $\mathbf{k}_1, \dots \mathbf{k}_n$ with $\mathbf{k} = \mathbf{k}_1 + \cdots + \mathbf{k}_n$ we have $\epsilon^L(\mathbf{k}) = D^L(\mathbf{k}_1) + \cdots + D^L(\mathbf{k}_n)$. This implies that the vector $(n!)^{-1/2} b_{\mathbf{k}_1}^* \cdots b_{\mathbf{k}_n}^* \Omega_{\alpha,\theta}$ is at the bottom of the spectrum of $\delta^{-1}H_{-1}^{\lambda,L} + H_0^{\lambda,L}$ in the sector of momentum $\mathbf{k}$. Again we can write down the perturbation expansion in terms of δ for the excitation spectrum, convergent for small δ:

$$\Psi^{\lambda,\delta,L}(\mathbf{k}) = \sum_{n=0}^{\infty} (\delta^n \Psi_n^{\lambda,L}(\mathbf{k}) + \delta^{n+\frac{1}{2}} \Psi_{n+\frac{1}{2}}^{\lambda,L}(\mathbf{k})), \quad \epsilon^{\lambda,\delta,L}(\mathbf{k}) = \sum_{n=-1}^{\infty} \delta^n \epsilon_n^{\lambda,L}(\mathbf{k}),$$

where $\Psi_0^{L,\lambda}(\mathbf{k}) = b_{\mathbf{k}}^* \Omega_{\alpha,\theta}$. Then we put $\delta = \lambda$ obtaining

$$\Psi^{\lambda,L}(\mathbf{k}) \sim \sum_{n=0}^{\infty} (\lambda^n \Psi_n^{\lambda,L}(\mathbf{k}) + \lambda^{n+\frac{1}{2}} \Psi_{n+\frac{1}{2}}^{\lambda,L}(\mathbf{k})), \quad \epsilon^{\lambda,L}(\mathbf{k}) \sim \sum_{n=-1}^{\infty} \lambda^n \epsilon_n^{\lambda,L}(\mathbf{k}). \tag{4.6}$$

Of course, we do not claim that the power series (4.5) and (4.6) have a nonzero radius of convergence. We only hope that they are in some sense asymptotic to the physical quantities.

We hope that the perturbation expansions (4.5) and (4.6) survive the thermodynamic limit. We do not expect that the nth terms of these expasions will be of order $O(\lambda^n)$. However, we hope that each next term will give a better approximation, as expressed in the following conjecture:

Conjecture 4.2. *(1) For any n, there exist*

$$\begin{aligned} e_n^\lambda &:= \lim_{L\to\infty} \frac{E_n^{\lambda,L}}{V}, \\ \epsilon_n^\lambda(\mathbf{k}) &:= \lim_{L\to\infty} \epsilon_n^{\lambda,L}(\mathbf{k}_L), \quad \mathbf{k}_L \to \mathbf{k}. \end{aligned}$$

(2)

$$\begin{aligned} \lim_{\lambda\searrow 0} e_{-1}^\lambda &= \frac{\mu^2}{2\hat{v}(\mathbf{0})}, \\ \lim_{\lambda\searrow 0} e_0^\lambda &= -\frac{1}{(2\pi)^d}\int \frac{1}{2}\left((\frac{1}{2}\mathbf{k}^2 + \hat{v}(\mathbf{k})\frac{\mu}{\hat{v}(\mathbf{0})}) - \omega_{\mathrm{bg},\mu}(\mathbf{k})\right) \mathrm{d}\mathbf{k}, \\ \lim_{\lambda\searrow 0} \epsilon_0^\lambda(\mathbf{k}) &= \epsilon_{\mathrm{bg}}(\mathbf{k}). \end{aligned}$$

(3) For some $0 < \sigma_1 < \sigma_2 \cdots$ with $\lim_{n\to\infty} \sigma_n = \infty$,

$$\begin{aligned} \lambda^n e_n^\lambda &= O(\lambda^{\sigma_n}), \quad n = 1, 2, \ldots \\ \lambda^n \epsilon_n^\lambda(\mathbf{k}) &= O(\lambda^{\sigma_n}), \quad n = 1, 2, \ldots. \end{aligned}$$

(4) For σ_n as above and all n,

$$\sum_{j=0}^{n} \lambda^j \epsilon_j^\lambda(\mathbf{0}) = O(\lambda^{\sigma_n}).$$

(1) is the existence of the thermodynamic limit of the perturbation expansion. (2) tells us that the lowest order terms in this expansion agree with the quantities obtained in the Bogoliubov approximation. (3) means that the later terms in the expansion are in some sense lower order than earlier. (4) says that there is no gap in the excitation spectrum at $\mathbf{k} = \mathbf{0}$.

It seems that a result similar to the above conjecture could be easier to prove than a result about the true energy density and the true infimum of the excitation spectrum.

Let us sum up the procedure that we propose to compute various quantities for Bose gas with λ small and fixed μ. We will call it the *Improved Bogoliubov Approach*

(1) Find a translation invariant squeezed state $\Omega_{\alpha,\theta}$ minimizing the expectation value of the Hamiltonian $H^{\lambda,L}$.
(2) Split the Hamiltonian as in (4.3):
$$H^{\lambda,L} = \lambda^{-1} H_{-1}^{\lambda,L} + H_0^{\lambda,L} + \sqrt{\lambda} H_{\frac{1}{2}}^{\lambda,L} + \lambda H_1^{\lambda,L}$$
according to the power in creation/annihilation operators adapted to $\Omega_{\alpha,\theta}$.
(3) Introduce a fictitious Hamiltonian with an additional coupling constant δ
$$H^{\lambda,\delta,L} = \delta^{-1} H_{-1}^{\lambda,L} + H_0^{\lambda,L} + \sqrt{\delta} H_{\frac{1}{2}}^{\lambda,L} + \delta H_1^{\lambda,L}.$$
(4) Compute the desired quantity perturbatively, obtaining a (formal) power series $c^{\lambda,\delta,L} = \sum_n \delta^n c_n^{\lambda,L}$.
(5) Go to the thermodynamic limit with each term in the series separately, obtaining $c_n^\lambda := \lim_{L\to\infty} c_n^{\lambda,L}$.
(6) Set $\delta = \lambda$, obtaining the power series $c^\lambda = \sum_n \lambda^n c_n^\lambda$, which is the final expression for the desired quantity.

4.3. **Approach with Isolated Condensate.** In the literature there are many works that are based on a somewhat different approach to the Bose gas with small λ and fixed μ. This approach is sometimes called the *Approach with Isolated Condensate*. We would like to compare it to the Improved Bogoliubov's Approach.

Let us describe the basic steps of this approach:

(1) Make the c-number substitution, obtaining the Hamiltonian $H^{\lambda,L}(\alpha)$ as in (3.12).
(2) Substitute $\alpha = \sqrt{\lambda^{-1}\kappa V}$ and split the Hamiltonian as
$$H^{\lambda,L}(\alpha) = \lambda^{-1}H_{-1}^{\kappa,L} + H_0^{\kappa,L} + \sqrt{\lambda}H_{\frac{1}{2}}^{\kappa,L} + \lambda H_1^{\kappa,L}.$$
according to the power of λ.
(3) Compute perturbatively the ground state energy, obtaining a (formal) power series $E^{\lambda,\kappa,L} = \sum_n \lambda^n E_n^{\kappa,L}$.
(4) Compute the desired quantity as a (formal) power series $c^{\lambda,\kappa,L} = \sum_n \lambda^n c_n^{\kappa,L}$.
(5) Minimize (up to the desired order in λ) $E^{\lambda,\kappa,L}$, obtaining $\kappa^{\lambda,L}$ as a function of λ, L.
(6) Substitute $\kappa^{\lambda,L}$ in the expression for the desired quantity, obtaining $c_n^{\lambda,L} = c_n^{\kappa^{\lambda,L},L}$.
(7) Go to the thermodynamic limit with each term of the series separately, obtaining $c_n^\lambda = \lim_{L\to\infty} c_n^{\lambda,L}$. The final expression for the desired quantity is
$$c^\lambda = \sum_n \lambda^n c_n^\lambda.$$

As proven by [22] (see Section 3.12), the Approach with Isolated Condensate is exact in the thermodynamic limit for the energy density. In the case of finer quantities, such as the infimum of the excitation spectrum or Green's functions, we do not see why the thermodynamic limit should make this approach exact.

Improved Bogoliubov Approach and Approach with Isolated Condensate seem to have a lot in common. In both of them the main step involves calculations with a quadratic Hamiltonian perturbed by 3rd and 4rth order perturbations. In both approaches the quadratic term does not contain a term linear in creation/annihilation operators. Note also that in both procedures the dependence of the final quantities on the coupling constant λ can be quite complicated, and not given just by a power series.

The Approach with Isolated Condensate may seem simpler technically, since the perturbation expansion is applied to a simpler splitting, whereas in the Improved Bogoliubov Approach the first step involves solving a complicated fixed point equation. It is however quite clear, that the Improved Bogoliubov Approach is physically better justified than the Approach with Isolated Condensate. In the former no term is dropped. In the latter, at the very beginning we drop an important term from the Hamiltonian.

5. Observables

In this section we work in the grand-canonical approach. We drop the subscript μ and L, so that H_μ^L is denoted by H. (In particular, in order not to clutter the notation we hide the dependence on L, which however plays an important role in what follows).

5.1. **Spontaneous symmetry breaking.** The Hamiltonian H is invariant with respect to the transformation generated by the number operator $\mathrm{e}^{\mathrm{i}\tau N}$. Consequently, its ground state can be chosen to have a definite number of particles.

It is however believed that in the thermodynamical limit this gauge invariance is spontaneously broken. (In fact, it is broken in the Bogoliubov method).

Let us try to describe this symmetry breaking rigorously. Following Bogoliubov [4], we perturb the Hamiltonian by a non-physical perturbation

$$H_\nu := H - \nu\sqrt{V}(a_{\mathbf{0}}^* + a_{\mathbf{0}}), \tag{5.1}$$

where $\nu > 0$. H_ν depends on the gauge:

$$\mathrm{e}^{\mathrm{i}\tau N}\, H_\nu\, \mathrm{e}^{-\mathrm{i}\tau N} = H - \nu\sqrt{V}(\mathrm{e}^{\mathrm{i}\tau}\, a_{\mathbf{0}}^* + \mathrm{e}^{-\mathrm{i}\tau}\, a_{\mathbf{0}}). \tag{5.2}$$

Let us assume that H_ν has a unique ground state given by the vector Ψ_ν. Note that the Hamiltonian H_ν is real, therefore we can assume Ψ_ν to be real as well. H_ν is translation invariant and the group of translations of the torus is compact. Hence we can take Ψ_ν to be translation invariant. The expectation value with respect to the vector Ψ_ν will be denoted

$$\langle\cdot\rangle_\nu := (\Psi_\nu | \cdot \Psi_\nu).$$

Because of the translation invariance we have

$$\begin{aligned} \langle a_{\mathbf{k}}\rangle_\nu &= 0, \quad \mathbf{k} \neq \mathbf{0}; \\ \langle a_{\mathbf{k}}^* a_{\mathbf{k}'}\rangle_\nu &= 0, \quad \mathbf{k} \neq \mathbf{k}'; \\ \langle a_{\mathbf{k}} a_{-\mathbf{k}'}\rangle_\nu &= 0, \quad \mathbf{k} \neq \mathbf{k}'. \end{aligned} \tag{5.3}$$

Thus the nontrivial one- and two-point correlation function are

$$\langle a_{\mathbf{0}}\rangle_\nu = \langle a_{\mathbf{0}}^*\rangle_\nu; \tag{5.4}$$

$$\langle a_{\mathbf{k}}^* a_{\mathbf{k}}\rangle_\nu = \langle a_{-\mathbf{k}}^* a_{-\mathbf{k}}\rangle_\nu; \tag{5.5}$$

$$\langle a_{\mathbf{k}} a_{-\mathbf{k}}\rangle_\nu = \langle a_{\mathbf{k}}^* a_{-\mathbf{k}}^*\rangle_\nu. \tag{5.6}$$

and the expressions (5.4), (5.5) and (5.6) are all real. Their reality follows from the reality of the Hamiltonian (5.1) and the reality of $\langle\cdot\rangle_\nu$.

Let us assume that there exists the limit

$$\langle\cdot\rangle := \lim_{\nu\searrow 0}\lim_{L\to\infty}\langle\cdot\rangle_\nu, \tag{5.7}$$

as a state on a suitable family $\mathfrak{A}$ of observables.

Clearly, $\mathfrak{A}$ is invariant with respect to the Hermitian conjugation. Moreover, the group of translations $\mathrm{e}^{\mathrm{i}\mathbf{x}P}\cdot\mathrm{e}^{-\mathrm{i}\mathbf{x}P}$ and the dynamics $\mathrm{e}^{\mathrm{i}\mathbf{x}H}\cdot\mathrm{e}^{-\mathrm{i}\mathbf{x}H}$ act on $\mathfrak{A}$.

Clearly, the ground state of $\mathrm{e}^{\mathrm{i}\tau N}\, H_\nu\, \mathrm{e}^{-\mathrm{i}\tau N}$ (before taking the thermodynamic limit) is given by $\mathrm{e}^{\mathrm{i}\tau N}\,\Psi_\nu$. Replacing Ψ_ν with $\mathrm{e}^{\mathrm{i}\tau N}\,\Psi_\nu$ and performing the limit (5.7), we obtain a new state on $\mathfrak{A}$. If (5.4) or (5.6) are non-zero, then this new state differs from $\langle\cdot\rangle_\nu$: (5.4) has to be multiplied with $\mathrm{e}^{\mathrm{i}\tau}$ and (5.6) with $\mathrm{e}^{\mathrm{i}2\tau}$.

Clearly, (5.3) are true if we replace $\langle\cdot\rangle_\nu$ with $\langle\cdot\rangle$. It is natural to assume that the following limits exist:

$$\rho := \lim_{\nu\searrow 0}\lim_{L\to\infty}\frac{\langle N\rangle_\nu}{V}; \tag{5.8}$$

$$\sqrt{\kappa} := \lim_{\nu\searrow 0}\lim_{L\to\infty}\frac{\langle a_{\mathbf{0}}\rangle_\nu}{\sqrt{V}}; \tag{5.9}$$

$$\langle a_{\mathbf{k}}^* a_{\mathbf{k}}\rangle = \lim_{\nu\searrow 0}\lim_{L\to\infty}\langle a_{\mathbf{k}}^* a_{\mathbf{k}}\rangle_\nu, \quad \mathbf{k}\neq\mathbf{0}; \tag{5.10}$$

$$\langle a_{\mathbf{k}} a_{-\mathbf{k}}\rangle = \lim_{\nu\searrow 0}\lim_{L\to\infty}\langle a_{\mathbf{k}} a_{-\mathbf{k}}\rangle_\nu, \quad \mathbf{k}\neq\mathbf{0}. \tag{5.11}$$

Clearly, the expressions (5.9), (5.10) and (5.11) are again real. All of them depend on μ. ρ is the density and κ can be interpreted as the density of the condensate.

5.2. **A priori estimates.** We will use notation explained in an abstract setting in Appendix H, where the reader will also find some general remarks about Green's functions and their motivation. In particular, for a pair of operators A, B the *static Green's function* is defined as

$$\langle\langle A, B\rangle\rangle_\nu \quad := \quad \langle A(H_\nu - E_\nu)^{-1}B\rangle_\nu + \langle B(H_\nu - E_\nu)^{-1}A\rangle_\nu .$$

Recall the operator

$$N_{\mathbf{q}} \quad := \quad \sum_{\mathbf{k}} a^*_{\mathbf{q}+\mathbf{k}} a_{\mathbf{k}} = \int \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}}\, a^*_{\mathbf{x}} a_{\mathbf{x}} \mathrm{d}\mathbf{x},$$

(see (3.5) and (2.13))

We will tacitly assume that we can perform the thermodynamic limit of various observables, such as

$$\begin{aligned}
\langle\langle a^*_{\mathbf{k}}, a_{\mathbf{k}}\rangle\rangle \quad &:= \quad \lim_{\nu\searrow 0}\lim_{L\to\infty} \langle\langle a^*_{\mathbf{k}}, a_{\mathbf{k}}\rangle\rangle_\nu ;\\
\langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle \quad &:= \quad \lim_{\nu\searrow 0}\lim_{L\to\infty} \langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle_\nu ;\\
s_{\mathbf{k}} \quad &:= \quad \lim_{\nu\searrow 0}\lim_{L\to\infty} \frac{\langle N^*_{\mathbf{k}} N_{\mathbf{k}}\rangle_\nu}{\langle N\rangle_\nu};\\
\chi_{\mathbf{k}} \quad &:= \quad \lim_{\nu\searrow 0}\lim_{L\to\infty} \frac{\langle\langle N^*_{\mathbf{k}}, N_{\mathbf{k}}\rangle\rangle_\nu}{\langle N\rangle_\nu}.
\end{aligned}$$

(Compare with the definition of $s_{\mathbf{k}}$ and $\chi_{\mathbf{k}}$ in (2.16) and (2.17)).

In this setting we have the following analog of (2.14):

$$\frac{1}{2}[N^*_{\mathbf{k}}, [H_\nu, N_{\mathbf{k}}]] = \frac{\mathbf{k}^2}{2} N + \frac{\nu\sqrt{V}}{2}(a_{\mathbf{0}} + a^*_{\mathbf{0}}). \tag{5.12}$$

It implies the so-called *f-sum rule*:

$$\frac{1}{2}\langle N^*_{\mathbf{k}}(H_\nu - E_\nu)N_{\mathbf{k}}\rangle_\nu + \frac{1}{2}\langle N_{\mathbf{k}}(H_\nu - E_\nu)N^*_{\mathbf{k}}\rangle_\nu = \frac{\mathbf{k}^2}{2}\langle N\rangle_\nu + \nu\sqrt{V}\langle a_{\mathbf{0}}\rangle_\nu. \tag{5.13}$$

By the Schwarz inequality and taking the thermodynamic limit, we obtain

$$s_{\mathbf{k}} \le \frac{1}{2}|\mathbf{k}|\sqrt{\chi_{\mathbf{k}}}. \tag{5.14}$$

In the theorem below, (5.16) is due to Pitaevski and Stringari [27, 34], and (5.17) is the zero-temperature version of the famous $\frac{1}{\mathbf{k}^2}$ Theorem of Bogoliubov [4].

Theorem 5.1.

$$\begin{aligned}
\langle a^*_{\mathbf{k}} a_{\mathbf{k}}\rangle \quad &\ge \quad \frac{\kappa}{4 s_{\mathbf{k}}\rho} - \frac{1}{2}, &(5.15)\\
&\ge \quad \frac{\kappa}{2|\mathbf{k}|\sqrt{\chi_{\mathbf{k}}}\rho} - \frac{1}{2}, &(5.16)\\
\langle\langle a_{\mathbf{k}}, a^*_{\mathbf{k}}\rangle\rangle \quad &\ge \quad \frac{\kappa}{\rho\mathbf{k}^2} + \left|\langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle + \frac{\kappa}{\rho\mathbf{k}^2}\right|. &(5.17)
\end{aligned}$$

Proof. To simplify the presentation, our proof will be not quite rigorous, since we will ignore ν and skip the thermodynamical limit involving $\lim\limits_{\nu\searrow 0}\lim\limits_{L\to\infty}$.

We set $A^* = a_{\mathbf{k}}$ and $B := N_{\mathbf{k}}$ in the uncertainty relation (G.2) and we obtain

$$\left(\langle a^*_{\mathbf{k}} a_{\mathbf{k}}\rangle + \frac{1}{2}\right)\langle N^*_{\mathbf{k}} N_{\mathbf{k}}\rangle \ge \frac{1}{4}|\langle a_{\mathbf{0}}\rangle|^2.$$

This proves (5.15). Now (5.14) implies (5.16).

To prove (5.17) introduce the operators

$$\begin{aligned} Q_{\mathbf{k}} &:= N_{\mathbf{k}} + N_{\mathbf{k}}^*, \\ R_{\mathbf{k}} &= \mathrm{i}[Q_{\mathbf{k}}, H]. \end{aligned}$$

We obtain

$$\begin{aligned} [Q_{\mathbf{k}}, [H, Q_{\mathbf{k}}]] &= 2\mathbf{k}^2 N - \mathbf{k}^2 Q_{2\mathbf{k}}, \\ [Q_{\mathbf{k}}, a_{\mathbf{k}}] &= -a_{\mathbf{0}} - a_{2\mathbf{k}}, \\ [Q_{\mathbf{k}}, a_{-\mathbf{k}}^*] &= a_{\mathbf{0}}^* + a_{-2\mathbf{k}}^*. \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{1}{2}\langle\langle R_{\mathbf{k}}, R_{\mathbf{k}}\rangle\rangle &= \frac{1}{2}\langle[Q_{\mathbf{k}}, [H, Q_{\mathbf{k}}]\rangle = \langle N\rangle \mathbf{k}^2, & (5.18) \\ \langle\langle a_{\mathbf{k}}, R_{\mathbf{k}}\rangle\rangle &= \mathrm{i}\langle[Q_{\mathbf{k}}, a_{\mathbf{k}}]\rangle = -\mathrm{i}\langle a_{\mathbf{0}}\rangle, & (5.19) \\ \langle\langle a_{-\mathbf{k}}^*, R_{\mathbf{k}}\rangle\rangle &= \mathrm{i}\langle[Q_{\mathbf{k}}, a_{-\mathbf{k}}^*]\rangle = \mathrm{i}\langle a_{\mathbf{0}}^*\rangle. & (5.20) \end{aligned}$$

(5.19) and (5.20) are sometimes called the *Bogoliubov sum rules* [4, 34].

For a complex parameter t we have

$$-\mathrm{i}\langle a_{\mathbf{0}}\rangle + \mathrm{i}t\langle a_{\mathbf{0}}^*\rangle = \langle\langle(a_{\mathbf{k}} + t a_{-\mathbf{k}}^*), R_{\mathbf{k}}\rangle\rangle. \tag{5.21}$$

We take the square of the absolute value of (5.21), apply (G.3), and we obtain

$$|\langle a_{\mathbf{0}}\rangle|^2 - t\langle a_{\mathbf{0}}^*\rangle^2 - \bar{t}\langle a_{\mathbf{0}}\rangle^2 + |t|^2|\langle a_{\mathbf{0}}\rangle|^2 \le \langle\langle(a_{\mathbf{k}} + t a_{-\mathbf{k}}^*), (a_{\mathbf{k}}^* + \bar{t} a_{-\mathbf{k}})\rangle\rangle\langle\langle R_{\mathbf{k}}, R_{\mathbf{k}}\rangle\rangle.$$

Taking into account (5.18), we obtain

$$\begin{aligned} 0 \le\; & \langle\langle a_{\mathbf{k}}, a_{\mathbf{k}}^*\rangle\rangle - \frac{|\langle a_{\mathbf{0}}\rangle|^2}{\langle N\rangle \mathbf{k}^2} \\ & + t\left(\langle\langle a_{-\mathbf{k}}^*, a_{\mathbf{k}}^*\rangle\rangle + \frac{\langle a_{\mathbf{0}}^*\rangle^2}{\langle N\rangle \mathbf{k}^2}\right) \\ & + \bar{t}\left(\langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle + \frac{\langle a_{\mathbf{0}}\rangle^2}{\langle N\rangle \mathbf{k}^2}\right) \\ & + |t|^2\left(\langle\langle a_{-\mathbf{k}}^*, a_{-\mathbf{k}}\rangle\rangle - \frac{|\langle a_{\mathbf{0}}\rangle|^2}{\langle N\rangle \mathbf{k}^2}\right). \end{aligned}$$

Using

$$\langle a_{\mathbf{0}}\rangle = \langle a_{\mathbf{0}}^*\rangle, \quad \langle\langle a_{-\mathbf{k}}^*, a_{-\mathbf{k}}\rangle\rangle = \langle\langle a_{\mathbf{k}}^*, a_{\mathbf{k}}\rangle\rangle, \quad \langle\langle a_{-\mathbf{k}}^*, a_{\mathbf{k}}^*\rangle\rangle = \langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle,$$

we obtain

$$\left|\langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle + \frac{\langle a_{\mathbf{0}}\rangle^2}{\langle N\rangle \mathbf{k}^2}\right|^2 \le \langle\langle a_{\mathbf{k}}^*, a_{\mathbf{k}}\rangle\rangle - \frac{|\langle a_{\mathbf{0}}\rangle|^2}{\langle N\rangle \mathbf{k}^2},$$

which implies (5.17). □

Note the following consequence of (5.17):

$$\langle\langle a_{\mathbf{k}}^*, a_{\mathbf{k}}\rangle\rangle - \langle\langle a_{\mathbf{k}}^*, a_{-\mathbf{k}}^*\rangle\rangle \ge \tfrac{2\kappa}{\rho\mathbf{k}^2}. \tag{5.22}$$

Theorem 5.2. *Let $\epsilon(\mathbf{k})$ be the IES at momentum $\mathbf{k}$. Then*

$$\begin{aligned} \epsilon(\mathbf{k})^2 \le\; & \frac{\mathbf{k}^2\rho}{2\kappa}\Big(\frac{\mathbf{k}^2}{2} - \mu + \rho\hat{v}(\mathbf{0}) & (5.23) \\ & + \frac{1}{2(2\pi)^d}\int \hat{v}(\mathbf{k})\left(2\langle a_{\mathbf{q}+\mathbf{k}}^* a_{\mathbf{q}+\mathbf{k}}\rangle + \langle a_{\mathbf{q}+\mathbf{k}}^* a_{-\mathbf{q}-\mathbf{k}}^*\rangle + \langle a_{\mathbf{q}+\mathbf{k}} a_{-\mathbf{q}-\mathbf{k}}\rangle\right)\mathrm{d}\mathbf{q}\Big), \\ \epsilon(\mathbf{k})^2 \le\; & \left(\frac{\mathbf{k}^2}{2}\right)^2 + 2\mathbf{k}^2\int \frac{|\mathbf{q}|^2}{2}\left\langle a_{\mathbf{q}}^* a_{\mathbf{q}}\right\rangle \mathrm{d}\mathbf{q} & (5.24) \\ & + \rho\int \mathrm{d}\mathbf{x}(1 - \cos\mathbf{k}\mathbf{x})\nabla_{\hat{\mathbf{k}}}^{(2)} v(\mathbf{x})\langle a_{\mathbf{0}}^* a_{\mathbf{x}}^* a_{\mathbf{x}} a_{\mathbf{0}}\rangle, \end{aligned}$$

where $\hat{\mathbf{k}}$ *denotes* $|\mathbf{k}|^{-1}\mathbf{k}$ *and* $\nabla_{\hat{\mathbf{k}}}^{(2)}v(\mathbf{x})$ *denotes the second derivative of* v *in the direction of* $\hat{\mathbf{k}}$.

Proof. To prove (5.23), we use (G.8) with $A^* = a_{\mathbf{k}} - a_{-\mathbf{k}}^*$ and $B = N_{\mathbf{k}}$ and then go to the thermodynamic limit.

To prove (5.24) we use (G.9) with $A = N_{\mathbf{k}}$ $\square$

Both estimates of Theorem (5.2) indicate the phononic character of the excitation spectrum. The estimate (5.23) is due to Wagner [39, 34]) and involves the symmetry breaking parameter κ. The estimate (5.24) involves the kinetic energy and the pair correlation function $\langle a_{\mathbf{0}}^* a_{\mathbf{x}}^* a_{\mathbf{x}} a_{\mathbf{0}}\rangle$ (here $\mathbf{0}$ refers to the position), but does not involve κ, hence it can be applied to situations without symmetry breaking. This estimate comes from [29, 25], see also [34].

5.3. **Green's functions of the Bose gas.** Let us consider two-point Green's functions of the Bose gas. We assume that $\langle\cdot\rangle$ is the state obtained by the limiting procedure in the thermodynamic limit, and we will ignore the complications due to the thermodynamic limit.

We define a 2×2 matrix of Green's functions

$$G(z,\mathbf{k}) := \begin{bmatrix} G_{11}(z,\mathbf{k}) & G_{21}(z,\mathbf{k}) \\ G_{12}(z,\mathbf{k}) & G_{22}(z,\mathbf{k}) \end{bmatrix},$$

$$\begin{aligned}
G_{11}(z,\mathbf{k}) &= \langle a_{\mathbf{k}}(H-E-z)^{-1}a_{\mathbf{k}}^*\rangle + \langle a_{\mathbf{k}}^*(H-E+z)^{-1}a_{\mathbf{k}}\rangle, \\
G_{21}(z,\mathbf{k}) &= \langle a_{-\mathbf{k}}^*(H-E-z)^{-1}a_{\mathbf{k}}^*\rangle + \langle a_{\mathbf{k}}^*(H-E+z)^{-1}a_{-\mathbf{k}}^*\rangle, \\
G_{12}(z,\mathbf{k}) &= \langle a_{\mathbf{k}}(H-E-z)^{-1}a_{-\mathbf{k}}\rangle + \langle a_{-\mathbf{k}}(H-E+z)^{-1}a_{\mathbf{k}}\rangle, \\
G_{22}(z,\mathbf{k}) &= \langle a_{-\mathbf{k}}^*(H-E-z)^{-1}a_{-\mathbf{k}}\rangle + \langle a_{-\mathbf{k}}(H-E+z)^{-1}a_{-\mathbf{k}}^*\rangle.
\end{aligned}$$

Note that, using the notation of Appendix H,

$$G_{ij}(z,\mathbf{k}) = G_{A_i,B_j}(z),$$

where $A_1 := a_{\mathbf{k}}$, $A_2 := a_{-\mathbf{k}}^*$ and $B_1 := a_{\mathbf{k}}^*$, $B_2 := a_{-\mathbf{k}}$. We use the conventions described in this appendix for the meaning of Green's functions both away from the real line and on the real line.

It is a general fact, which does not depend on the details of the system, that

$$\begin{aligned}
G_{11}(z,\mathbf{k}) &= \overline{G_{11}(\overline{z},\mathbf{k})} &= G_{22}(-z,-\mathbf{k}), \\
G_{12}(z,\mathbf{k}) &= \overline{G_{21}(\overline{z},\mathbf{k})} &= G_{12}(-z,-\mathbf{k}).
\end{aligned}$$

By the reflection invariance of the Bose gas

$$G_{ij}(z,\mathbf{k}) = G_{ij}(z,-\mathbf{k}). \tag{5.25}$$

Obviously, for any observable A, $\langle A^*\rangle = \overline{\langle A\rangle}$. But the state $\langle\cdot\rangle$ is real, hence $\overline{\langle A\rangle} = \langle\,\overline{A}\,\rangle$. Note also that $H = \overline{H}$, $a_{\mathbf{k}} = \overline{a}_{\mathbf{k}}$. Therefore,

$$G_{12}(z,\mathbf{k}) = G_{21}(z,\mathbf{k}).$$

Note that $G_{11}(0,\mathbf{k}) = \langle\langle a_{\mathbf{k}}^*, a_{\mathbf{k}}\rangle\rangle$ and $G_{12}(0,\mathbf{k}) = \langle\langle a_{\mathbf{k}}, a_{-\mathbf{k}}\rangle\rangle$, hence by (5.22)

$$G_{11}(0,\mathbf{k}) - G_{12}(0,\mathbf{k}) \geq \frac{c}{\mathbf{k}^2}. \tag{5.26}$$

Let us introduce the "full mass operator"

$$\begin{aligned}
&\Sigma(z,\mathbf{k}) \\
= &\begin{bmatrix} \Sigma_{11}(z,\mathbf{k}) & \Sigma_{12}(z,\mathbf{k}) \\ \Sigma_{21}(z,\mathbf{k}) & \Sigma_{22}(z,\mathbf{k}) \end{bmatrix} := \frac{1}{2\pi}\begin{bmatrix} G_{11}(z,\mathbf{k}) & G_{12}(z,\mathbf{k}) \\ G_{21}(z,\mathbf{k}) & G_{22}(z,\mathbf{k}) \end{bmatrix}^{-1} \\
= &\frac{1}{2\pi}\left(G_{11}(z,\mathbf{k})G_{22}(z,\mathbf{k}) - G_{12}(z,\mathbf{k})G_{21}(z,\mathbf{k})\right)^{-1}\begin{bmatrix} G_{22}(z,\mathbf{k}) & -G_{12}(z,\mathbf{k}) \\ -G_{21}(z,\mathbf{k}) & G_{11}(z,\mathbf{k}) \end{bmatrix}.
\end{aligned}$$

Consequently,

$$\Sigma_{11}(0,\mathbf{k}) - \Sigma_{12}(0,\mathbf{k}) \quad = \quad \frac{1}{2\pi\left(G_{11}(0,\mathbf{k}) - G_{12}(0,\mathbf{k})\right)}.$$

(5.26) implies

$$\frac{\mathbf{k}^2}{2\pi c} \geq \Sigma_{11}(0,\mathbf{k}) - \Sigma_{12}(0,\mathbf{k}) \geq 0,$$

and in particular

$$\Sigma_{11}(0,\mathbf{0}) - \Sigma_{12}(0,\mathbf{0}) \quad = \quad 0. \tag{5.27}$$

(5.27) was first proven in the framework of perturbation theory for the Bose gas with isolated condensate, and is sometimes called the Hugenholz-Pines Theorem, [14], see also [9]. The proof that we present is valid for the correct Hamiltonian of the Bose gas and is due to Bogoliubov [4].

Note that (5.27) implies that $G(z,\mathbf{k})$ has a singularity at $(z,\mathbf{k}) = (0,\mathbf{0})$, which is an argument for the absence of a gap in the excitation spectrum. Bogoliubov [4] gives also an argument for the phononic shape of the excitation spectrum. The argument is based on the assumption that $\Sigma(z,\mathbf{k})$ is regular in z, $\mathbf{k}$ around $(0,\mathbf{0})$. Note that

$$\det\Sigma(z,\mathbf{k}) \quad = \quad \Sigma_{11}(z,\mathbf{k})\Sigma_{22}(z,\mathbf{k}) - \Sigma_{12}(z,\mathbf{k})\Sigma_{21}(z,\mathbf{k})$$

is invariant with respect to the transformations $\mathbf{k} \mapsto -\mathbf{k}$ and $z \mapsto -z$. Finally, by (5.27), we know that $\Sigma(0,\mathbf{0}) = 0$. Therefore,

$$\det\Sigma(z,\mathbf{k}) \quad = \quad \gamma z^2 + \beta\mathbf{k}^2 + O(|z|^4 + |\mathbf{k}|^4).$$

We have $\overline{\det\Sigma(z,\mathbf{k})} = \det\Sigma(\overline{z},\mathbf{k})$. Hence γ and β are real as well. For purely imaginary nonzero z, $\det\Sigma(z,\mathbf{k})$ is nonzero. Hence γ and β cannot have the same sign. Therefore, $\delta = -\frac{\beta}{\gamma} \geq 0$.

Assume now that β, γ are not zero. Then $0 < \delta < \infty$, and

$$\det\Sigma(\sqrt{\delta}|\mathbf{k}|, \mathbf{k}) = O(|\mathbf{k}|^4).$$

Hence, for small $\omega, \mathbf{k}$, the Green's function $G(\omega,\mathbf{k})$ has a sharp peak along $\omega(\mathbf{k}) = \sqrt{\delta}|\mathbf{k}|$.

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. The excitation spectrum of (A.1) is not arbitrary – it has to be a subadditive function. This appendix describes a number of easy results about subadditive functions. They are quite straightforward and probably they mostly belong to the folk wisdom. However, we have never seen them explicitly described in the literature, and we believe them to be relevant for physical properties of Bose gas.

The Hamiltonian of interacting Bose gas is not purely quadratic. Nevertheless, some arguments indicate that the infimum of its excitation spectrum in the thermodynamic limit is subadditive. A heuristic argument in favor of this conjecture is described in the next appendix.

Even if one questions this argument, there exists another motivation for a study of subadditive functions. Quadratic Hamiltonians are often used in statistical physics as approximate effective Hamiltonians. In particular, this is the case of the Bogoliubov Hamiltonian H_{bg}.

We will show that there exists a large class of subadditive functions with the properties properties described by Conjecture 1.1 or 3.4, (3) or (3)', and (4) (which correspond to the superfluidity or periodicity, and to a finite speed of sound). We will also show that if the elementary excitations possess these properties, then so does the IES.

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 hull 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 $\epsilon(\mathbf{k})$ its subadditive hull, then $\epsilon(\mathbf{k})$ is the infimum of its excitation spectrum.

Let us state and prove some facts about subadditive functions and subadditive hulls, 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 hull 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 two theorems, which easily follow from Theorems A.1, A.2 and A.3:

Theorem A.4. *Suppose that $\omega \geq 0$ is a spherically symmetric function on $\mathbb{R}^d$ and ϵ is its subadditive hull.*

(1) ϵ is spherically symmetric.
(2) If $\inf\limits_{\mathbf{k}\neq\mathbf{0}} \frac{\omega(\mathbf{k})}{|\mathbf{k}|} = c$, then $\inf\limits_{\mathbf{k}\neq\mathbf{0}} \frac{\epsilon(\mathbf{k})}{|\mathbf{k}|} = c$.
(3) If $\liminf_{\mathbf{k}\to\mathbf{0}} \frac{\omega(\mathbf{k})}{|\mathbf{k}|} = c$, then $\epsilon(\mathbf{k}) \leq c|\mathbf{k}|$.
(4) Suppose that for some $c > 0$, we have $\omega(\mathbf{k}) \geq c\min(|\mathbf{k}|, 1)$. Then

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

Theorem A.5. *Suppose that $\omega \geq 0$ is an even function on $\mathbb{R}$ periodic with respect to $\mathbb{Z}$. Let ϵ be its subadditive hull.*

(1) $\epsilon(\mathbf{k})$ is even and periodic with respect to $\mathbb{Z}$.
(2) If, for some $c > 0$, we have $\omega(\mathbf{k}) \geq c\mathrm{dist}(\mathbf{k}, \mathbb{Z})$, then

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

Appendix B. Subadditivity of the excitation spectrum of interacting Bose gas

In this appendix we describe a heuristic argument in favor of Conjecture 3.4 (5). Recall that this conjecture says that the IES of interacting Bose gas in the thermodynamic limit should be subadditive. Clearly, this would be true if the Bose gas was described by a quadratic Hamiltonian of a form A.1. We will see, however, that this conjecture follows as well from an assumption saying that one can describe excitations by approximately localized operators.

Consider Bose gas in a box of side length L where L is very large. Let Φ_0 be the ground state of the Hamiltonian and E_0 its ground state energy, so that $H\Phi_0 = E_0\Phi_0$ and $P\Phi_0 = 0$. Let $(E_0 + e_i, \mathbf{k}_i) \in \mathrm{sp}(H, P)$, $i = 1, 2$. We can find eigenvectors with these eigenvalues, that is, vectors Φ_i satisfying $H\Phi_i = (E_0+e_i)\Phi_i$, $P\Phi_i = \mathbf{k}_i\Phi_i$. Let us make the assumption that it is possible to find operators A_i, which are polynomials in creation and annihilation operator smeared with functions well localized in configuration space such that $PA_i \approx A_i(P + \mathbf{k}_i)$, and which approximately create the vectors Φ_i from the ground state, that is $\Phi_i \approx A_i\Phi_0$. (Note that here a large size of L plays a role). By replacing Φ_2 with $\mathrm{e}^{\mathrm{i}\mathbf{y}P}\,\Phi_2$ for some $\mathbf{y}$ and A_2 with $\mathrm{e}^{\mathrm{i}\mathbf{y}P}\,A_2\,\mathrm{e}^{-\mathrm{i}\mathbf{y}P}$, we can make sure that the regions of localization of A_1 and A_2 are separated by a large distance.

Now consider the vector $\Phi_{12} := A_1A_2\Phi_0$. Clearly,

$$P\Phi_{12} \approx (\mathbf{k}_1 + \mathbf{k}_2)\Phi_{12}.$$

Φ_{12} looks like the vector Φ_i in the region of localization of A_i, elsewhere it looks like Φ_0. The Hamiltonian H involves only expressions of short range (the potential decays in space). Therefore, we expect that

$$H\Phi_{12} \approx (E_0 + e_1 + e_2)\Phi_{12}.$$

If this is the case, it implies that $(E_0 + e_1 + e_2, \mathbf{k}_1 + \mathbf{k}_2) \in \mathrm{sp}(H, P)$, and hence it shows that the IES is subadditive.

Clearly, the argument we presented has its weak points – it is based on approximate locality, which can be violated because of correlations due to the Bose-Einstein condensation. Nevertheless, we have the impression that many physicists believe that even in the interacting case, in the thermodynamic limit, one can often "compose excitations" in a sense similar to the one described above. (See the discussion of the concept of elementary excitations in interacting systems by Lieb [19], and the experimental paper [24]).

Appendix C. Speed of sound at zero temperature

It is well known (e.g. [12]) that at any temperature the speed of sound is given by

$$c_{\mathrm{s}} = \sqrt{\frac{\partial p}{\partial \rho}\Big|_S},$$

where p is the pressure, ρ is the density and S is the entropy. (Recall that we assume that the mass of an individual particle is 1).

Let E denote the ground state energy (which corresponds to the total energy at zero temperature), V the volume and n the number of particles. Note that $n = V\rho$ and $E = Ve(\rho)$, where $e(\rho)$ denotes the energy density. At zero temperature the pressure is given by

$$p = -\frac{\partial E}{\partial V}\Big|_n = -e(\rho) + \rho e'(\rho).$$

Clearly, at zero temperature the entropy is zero. Therefore,

$$\begin{aligned} c_{\mathrm{s}}^2 &= \frac{\partial p}{\partial \rho}\Big|_{S=0} = \frac{\partial p}{\partial \rho}\Big|_{T=0} \\ &= \frac{\partial}{\partial \rho}\left(-e(\rho) + \rho e'(\rho)\right) = \rho e''(\rho). \end{aligned}$$

Appendix D. Wick and anti-Wick symbol

Let $a_1^*, a_2^*, \dots, a_n^*$ and $a_1, a_2, \dots, a_n$ be creation/annihilation operators. Let H be an operator given as a polynomial in these operators. We can write H in two ways:

$$H = \sum_{\gamma,\delta} h_{\gamma,\delta}(a^*)^\gamma a^\delta = \sum_{\gamma,\delta} \tilde{h}_{\gamma,\delta} a^\delta (a^*)^\gamma.$$

(We use here the multiindex notation, e.g. $a^\alpha = a_1^{\alpha_1} \cdots a_n^{\alpha_n}$). Then the function

$$\mathbb{C}^n \ni \alpha \mapsto H(\alpha) = \sum_{\gamma,\delta} h_{\gamma,\delta} \overline{\alpha}^\gamma \alpha^\delta$$

is called the *Wick symbol* of the operator H. (Synonyms: lower symbol, normal symbol, covariant symbol, a^*, a-symbol, Q-representation). The function

$$\mathbb{C}^n \ni \alpha \mapsto \tilde{H}(\alpha) = \sum_{\gamma,\delta} \tilde{h}_{\gamma,\delta} \overline{\alpha}^\gamma \alpha^\delta$$

is called the *anti-Wick symbol* of the operator H. (Synonyms: upper symbol, antinormal symbol, contravariant symbol, a, a^*-symbol, P-representation).

Introduce the standard coherent states:

$$W(\alpha) := \exp\left(\sum_{i=1}^n (-\alpha_i a_i^* + \overline{\alpha}_i a_i)\right), \quad \Omega_\alpha := W(\alpha)\Omega.$$

Note the identities (that can be used as alternative definitions of the Wick and anti-Wick symbols):

$$H(\alpha) = (\Omega_\alpha | H\Omega_\alpha), \tag{D.1}$$

$$H = \int_{\mathbb{C}} \tilde{H}(\alpha)|\Omega_\alpha)(\Omega_\alpha|\frac{\mathrm{d}^2\alpha}{\pi}. \tag{D.2}$$

Let H be a bounded from below self-adjoint operator. We have the following lower and upper bound for the ground state energy of H, which follow immediately from (D.1) and (D.2):

$$\inf\{\tilde{H}(\alpha)\ :\ \alpha \in \mathbb{C}^n\} \leq \inf \mathrm{sp} H \leq \inf\{H(\alpha)\ :\ \alpha \in \mathbb{C}^n\}. \tag{D.3}$$

Appendix E. 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

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

Then

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

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

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

Then

$$\begin{aligned} U_\theta a U_\theta^* &= \cosh|\theta| a + \tfrac{\theta}{|\theta|} \sinh|\theta| a^*, \\ U_\theta a^* U_\theta^* &= \cosh|\theta| a^* + \tfrac{\overline{\theta}}{|\theta|} \sinh|\theta| a, \\ U_\theta^* \Omega &= (1 + \tanh^2|\theta|)^{\frac{1}{4}} \mathrm{e}^{-\frac{\theta}{2|\theta|} \tanh|\theta| a^* a^*} \Omega. \end{aligned}$$

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

Appendix F. Computations of the Bogoliubov rotation

In this appendix we give the computations of the rotated terms in the Hamiltonian used in Section 3.4.

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

$$\begin{aligned}
U_\theta a^*_{\mathbf{k}+\mathbf{k}'} a_{\mathbf{k}} a_{\mathbf{k}'} U^*_\theta \quad = \quad & \big(c_{\mathbf{0}}(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + \overline{s}_{\mathbf{0}} c_{\mathbf{k}} s_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a_{\mathbf{0}} \\
& - \big(s_{\mathbf{0}}(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + c_{\mathbf{0}} \overline{c}_{\mathbf{k}} s_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a^*_{\mathbf{0}} \\
& + \text{higher order terms;} \\
U_\theta a_{\mathbf{k}+\mathbf{k}'} a^*_{\mathbf{k}} a^*_{\mathbf{k}'} U^*_\theta \quad = \quad & \big(c_{\mathbf{0}}(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + s_{\mathbf{0}} c_{\mathbf{k}} \overline{s}_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a^*_{\mathbf{0}} \\
& - \big(\overline{s}_{\mathbf{0}}(|s_{\mathbf{k}}|^2\delta(\mathbf{k}') + |s_{\mathbf{k}'}|^2\delta(\mathbf{k})) + c_{\mathbf{0}} c_{\mathbf{k}} \overline{s}_{\mathbf{k}} \delta(\mathbf{k}+\mathbf{k}')\big)\, a_{\mathbf{0}} \\
& + \text{higher order terms;}
\end{aligned}$$

$$\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 \\
= \quad & 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) \\
+ \quad & |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) \\
+ \quad & \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) \\
+ \quad & \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)\Big) \\
& + \text{higher order terms.}
\end{aligned}$$

Appendix G. Operator inequalities

Let us fix a vector Ψ and let $\langle A \rangle$ denote $(\Psi|A\Psi)$. Let $[A,B]_+ := AB + BA$ denote the anticommutator. Occasionally, we will write $[A,B]_- := AB - BA$ for the usual commutator.

Theorem G.1. *Suppose that A, B are operators. We have the following inequalities:*

(1) **Schwarz inequality for an anticommutator**

$$|\langle [A^*, B]_+ \rangle|^2 \le \langle [A^*, A]_+ \rangle \langle [B^*, B]_+ \rangle. \tag{G.1}$$

(2) **Uncertainty relation for a pair of operators**

$$|\langle [A^*, B] \rangle|^2 \le \langle [A, A^*]_+ \rangle \langle [B, B^*]_+ \rangle. \tag{G.2}$$

Proof. We add the inequalities

$$0 \le (A + tB)^*(A + tB), \quad 0 \le (A \pm tB)(A \pm tB)^*,$$

obtaining

$$0 \le [A, A^*]_+ + \overline{t}[B^*, A]_\pm + t[A^*, B]_\pm + |t|^2 [B^*, B]_+.$$

Then we take the expectation value of both sides and set $t = -\frac{\langle [B^*, A]_\pm \rangle}{\langle [B^*, B]_+ \rangle}$. □

Suppose that H is an operator bounded from below and Ψ is its ground state vector:

$$H\Psi = E\Psi, \quad H - E \ge 0.$$

Assume that $\langle A \rangle = \langle B \rangle = 0$. Then we will write

$$\langle\langle A, B \rangle\rangle := \langle A(H-E)^{-1}B \rangle + \langle B(H-E)^{-1}A \rangle.$$

Theorem G.2.

$$|\langle\langle A^*, B\rangle\rangle|^2 \leq \langle\langle A^*, A\rangle\rangle\langle\langle B^*, B\rangle\rangle; \tag{G.3}$$

$$|\langle [A^*, B]\rangle|^2 \leq \langle\langle A^*, A\rangle\rangle\langle [B^*, [H, B]]\rangle. \tag{G.4}$$

Proof. To see (G.3) we apply the Schwarz inequality to the positive definite form $\langle\langle A^*, B\rangle\rangle$.

To obtain (G.4) we first use the identity

$$\langle [A^*, B]\rangle = \langle\langle A^*, [H, B]\rangle\rangle, \tag{G.5}$$

and then (G.3). □

Theorem G.3. *Let $\mathcal{H}_0$ be the space*

$$\mathcal{H}_0 := \{f_1(H)A\Psi + g(H)A^*\Psi \ : \ f, g\}^{\mathrm{cl}}$$

(the smallest invariant subspace of the operator H containing $A\Psi$ and $A^*\Psi$). Let $\epsilon := \inf \mathrm{sp} H\Big|_{\mathcal{H}_0} - E$. Then

$$\epsilon \leq \frac{\langle [A^*, [H, A]]\rangle}{\langle [A^*, A]_+\rangle}, \tag{G.6}$$

$$\epsilon^2 \leq \frac{\langle [A^*, [H, A]]\rangle}{\langle\langle A^*, A\rangle\rangle}, \tag{G.7}$$

$$\epsilon^2 \leq \frac{\langle [A^*, [H, A]]\rangle\langle [B^*, [H, B]]\rangle}{|\langle [A^*, B]\rangle|^2}, \tag{G.8}$$

$$\epsilon^2 \leq \frac{\langle [[A^*, H][H, [H, A]]]\rangle}{\langle [A^*, [H, A]]\rangle}. \tag{G.9}$$

Proof. To prove (G.6) we add

$$\epsilon\langle A^*A\rangle \leq \langle A^*(H - E)A\rangle, \quad \epsilon\langle AA^*\rangle \leq \langle A(H - E)A^*\rangle.$$

To prove (G.7) we add

$$\epsilon^2\langle A^*(H - E)^{-1}A\rangle \leq \langle A^*(H - E)A\rangle, \ \ \epsilon^2\langle A(H - E)^{-1}A^*\rangle \leq \langle A(H - E)A^*\rangle.$$

(G.8) follows from (G.7) and (G.4). □

(G.6) is called the Feynman bound [34] and (G.8) is due to Wagner [39, 34]. (G.9) comes from [29, 25].

Appendix H. Green's functions

We consider a quantum system described by a bounded from below Hamiltonian H. We assume that it has a unique ground state $(\Psi| \cdot \Psi) = \langle\cdot\rangle$, $H\Psi = E\Psi$. If A is an operator, then we will write

$$A(t) := \mathrm{e}^{\mathrm{i}tH} A\, \mathrm{e}^{-\mathrm{i}tH}.$$

The *time-dependent Green's* function associated to a pair of operators A, B is defined as the function depending on $t \in \mathbb{R}$

$$\begin{aligned} G^{\mathrm{td}}_{A,B}(t) &= \theta(-t)\langle A(0)B(t)\rangle + \theta(t)\langle B(t)A(0)\rangle \\ &= \theta(-t)\langle A\, \mathrm{e}^{\mathrm{i}t(H-E)} B\rangle + \theta(t)\langle B\, \mathrm{e}^{-\mathrm{i}t(H-E)} A\rangle, \end{aligned} \tag{H.1}$$

where θ is the Heaviside function.

We also introduce the *energy-dependent Green's function*, which is the Fourier transform of (H.1) (with one of conventional normalizations). It is the distribution on $\omega \in \mathbb{R}$ defined as

$$\begin{aligned} G_{A,B}(z) &= \lim_{\epsilon \searrow 0} \mathrm{i} \int G_{A,B}(t)\, \mathrm{e}^{-\mathrm{i}\omega t - \epsilon |t|}\, \mathrm{d}t \\ &= \lim_{\epsilon \searrow 0} \mathrm{i} \int_0^\infty \Big(\langle A\, \mathrm{e}^{-\mathrm{i}t(H-E-\omega-\mathrm{i}\epsilon)}\, B \rangle + \langle B\, \mathrm{e}^{\mathrm{i}t(H-E+\omega-\mathrm{i}\epsilon)}\, A \rangle \Big)\, \mathrm{d}t \\ &= \langle A(H-E-\omega-\mathrm{i}0)^{-1}B \rangle + \langle B(H-E+\omega-\mathrm{i}0)^{-1}A \rangle. \end{aligned} \tag{H.2}$$

Finally, the *analytic Green's function* is defined for $z \in \mathbb{C} \setminus (\mathrm{sp}(H-E) \cup \mathrm{sp}(E-H))$ and is defined as

$$G^{\mathrm{an}}_{A,B}(z) = \langle A(H-E-z)^{-1}B \rangle + \langle B(H-E+z)^{-1}A \rangle.$$

The distribution $G_{A,B}(\omega)$ is the boundary value of the analytic function $G^{\mathrm{an}}_{A,B}(z)$, provided that we approach the the real line from the appropriate side. Besides, in the energy gap both functions coincide:

$$\begin{aligned} G_{A,B}(\omega) &= G^{\mathrm{an}}_{A,B}(\omega - \mathrm{i}0), \quad \omega \in \mathrm{sp}(E-H) \subset]-\infty, 0]; \\ G_{A,B}(\omega) &= G^{\mathrm{an}}_{A,B}(\omega), \qquad \omega \in \mathbb{R} \setminus \{\mathrm{sp}(H-E) \cup \mathrm{sp}(E-H)\}; \\ G_{A,B}(\omega) &= G^{\mathrm{an}}_{A,B}(\omega + \mathrm{i}0), \quad \omega \in \mathrm{sp}(H-E) \subset]0, \infty]. \end{aligned}$$

Motivated by the above relations, following the usual convention, we can treat $G_{A,B}(\omega)$ and $G^{\mathrm{an}}_{A,B}(z)$ as restrictions of a single fuction and drop the subscript an. Note that

$$G_{A,B}(z) = \overline{G_{B^*,A^*}(\overline{z})} = G_{B,A}(-z).$$

Green's functions are well motivated physically. Let us briefly describe their two separate physical applications.

Following [4], let us first describe the physical meaning of the *static* Green's function

$$G_{A,B}(0) = \langle\langle A, B \rangle\rangle.$$

Suppose that Ψ is an eigenvector of H (not necessarily a ground state). Let B be a perturbation with $1_{\{E\}}(H)B\Psi = 0$. Suppose that it is possible to apply perturbation theory to the family $H_\tau := H + \tau B$ obtaining an analytic familly of eigenvectors Ψ_τ with eigenvalues E_τ such that $E_0 = E$ and $\Psi_0 = \Psi$. The Rayleigh-Schrödinger perturbation theory says that

$$\Psi_\tau = \Psi + \tau(H-E)^{-1}B\Psi + O(\tau^2). \tag{H.3}$$

Let $\langle A \rangle_\tau := (\Psi_\tau | A \Psi_\tau)$. (H.3) implies that for any operator A we have

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \langle A \rangle_\tau \Big|_{\tau=0} = \langle\langle B, A \rangle\rangle. \tag{H.4}$$

Thus $\langle\langle A, B \rangle\rangle$ measures the linear response of eigenvalues of a quantum system.

Let us describe a typical illustration of the physical meaning of $G_{A,B}(z)$ for a general z. Suppose that at time 0 the system described by a Hamiltonian H is in its ground state. We perturb the Hamiltonian by a weak perturbation λB and at time t we measure the observable A. The shift of the expectation of the measurement is

$$\begin{aligned} \delta_\lambda(t) &:= \langle \mathrm{e}^{\mathrm{i}t(H+\lambda B)}\, A\, \mathrm{e}^{-\mathrm{i}t(H+\lambda B)} \rangle - \langle A \rangle \\ &\approx \mathrm{i}\lambda \int_0^t \mathrm{d}u \langle [B(u), A(t)] \rangle \\ &= \mathrm{i}\lambda \int_0^t \mathrm{d}s\, \Big(\langle B\, \mathrm{e}^{\mathrm{i}s(H-E)}\, A \rangle - \langle A\, \mathrm{e}^{-\mathrm{i}s(H-E)}\, B \rangle \Big), \end{aligned}$$

where we took the leading term in λ. For some $\mathrm{Im} z < 0$, we compute the Laplace transform of $\delta_\lambda(t)$, make the linear approximation and change the variable $u = t - s$:

$$\begin{aligned}
\int_0^\infty \mathrm{e}^{-\mathrm{i}tz}\,\delta_\lambda(t)\mathrm{d}t &\approx \mathrm{i}\lambda \int_0^\infty \mathrm{e}^{-\mathrm{i}tz}\,\mathrm{d}t \int_0^t \Big(\langle B\,\mathrm{e}^{\mathrm{i}s(H-E)}\,A\rangle - \langle A\,\mathrm{e}^{-\mathrm{i}s(H-E)}\,B\rangle \Big)\,\mathrm{d}s \\
&= \mathrm{i}\lambda \int_0^\infty \mathrm{e}^{-\mathrm{i}uz}\,\mathrm{d}u \int_0^\infty \Big(\langle B\,\mathrm{e}^{\mathrm{i}s(H-E-z)}\,A\rangle - \langle A\,\mathrm{e}^{-\mathrm{i}s(H-E+z)}\,B\rangle \Big)\,\mathrm{d}s \\
&= \frac{\mathrm{i}\lambda}{z} G_{B,A}(z).
\end{aligned}$$

Thus, $G_{A,B}(z)$ measures the *linear response* of the dynamics a quantum system.

H.1. **The van Hove formfactor.** A typical experiment measuring excitation spectrum involves scattering with a beam of particles, typically neutrons. Following van Hove [38], let us try to describe such an experiment mathematically.

We can assume that a neutron of mass m interacts with each particle of the Bose gas through a potential w. Its incident momentum is $\mathbf{p}_\mathrm{i}$. We measure scattered neutrons of momentum $\mathbf{p}_\mathrm{f} \neq \mathbf{p}_\mathrm{i}$. The space describing the Bose gas and a single neutron is $\Gamma_\mathrm{s}(\Lambda) \otimes L^2(\mathbb{R}^d)$ and the Hamiltonian is

$$\begin{aligned}
\tilde{H}_\lambda &:= \tilde{H}_0 + \lambda I \\
&= H \otimes \mathbb{1} + \mathbb{1} \otimes \frac{1}{2m} D_\mathbf{y}^2 + \lambda \int a_\mathbf{x}^* a_\mathbf{x} w(\mathbf{x} - \mathbf{y})\mathrm{d}\mathbf{x},
\end{aligned}$$

where $\mathbf{y}$ denotes the position of the neutron, $D_\mathbf{y}$ its momentum, λ is small, and as usual H is the Hamiltonian of the Bose gas. Let $\Phi_\mathbf{p}$ denote the plane wave function of momentum $\mathbf{p}$, that is $\Phi_\mathbf{p}(\mathbf{y}) = V^{-\frac{1}{2}}\,\mathrm{e}^{\mathrm{i}\mathbf{p}\mathbf{y}}$.

Suppose that the initial state of the composite system is $\Psi \otimes \Phi_{\mathbf{p}_\mathrm{i}}$, where Ψ is the ground state. Let E be the ground state energy and $\sigma_\mathrm{i} = \frac{1}{2m}\mathbf{p}_\mathrm{i}^2$ the energy of the incident neutron. After time $2T$ the evolved state is given by

$$\begin{aligned}
\Theta(T, \mathbf{p}_\mathrm{i}) &= \mathrm{e}^{-\mathrm{i}2T\tilde{H}_\lambda}\,\Psi \otimes \Phi_{\mathbf{p}_\mathrm{i}} \\
&\approx \mathrm{e}^{-\mathrm{i}2T\tilde{H}_0}\,\Psi \otimes \Phi_{\mathbf{p}_\mathrm{i}} \\
&\quad -\mathrm{i}\lambda \int_0^{2T} \mathrm{e}^{-\mathrm{i}2T\tilde{H}_0 + \mathrm{i}t(\tilde{H}_0 - E - \sigma_\mathrm{i})}\,I\mathrm{d}t\Psi \otimes \Phi_{\mathbf{p}_\mathrm{i}} \\
&= \mathrm{e}^{-\mathrm{i}2T(E+\sigma_\mathrm{i})}\,\Psi \otimes \Phi_{\mathbf{p}_\mathrm{i}} \\
&\quad -2\mathrm{i}\lambda\,\mathrm{e}^{-\mathrm{i}T(\tilde{H}_0 + E + \sigma_\mathrm{i})}\,\frac{\sin T(\tilde{H}_0 - E - \sigma_\mathrm{i})}{\tilde{H}_0 - E - \sigma_\mathrm{i}} I\Psi \otimes \Phi_{\mathbf{p}_\mathrm{i}},
\end{aligned}$$

where we used the so-called Born approximation. Let $\sigma_\mathrm{f} := \frac{1}{2m}\mathbf{p}_\mathrm{f}^2$ be the final energy of the neutron. We introduce also the momentum and energy transfer

$$\mathbf{q} = \mathbf{p}_\mathrm{i} - \mathbf{p}_\mathrm{f}, \quad \omega := \sigma_\mathrm{i} - \sigma_\mathrm{f}.$$

To obtain the amplitude of the measurement of the momentum $\mathbf{p}_\mathrm{f}$ we take the partial scalar product of $\Theta(T, \mathbf{p}_\mathrm{i}) \in \Gamma_\mathrm{s}(\Lambda) \otimes L^2(\mathbb{R}^d)$ with with $\Phi_{\mathbf{p}_\mathrm{f}} \in L^2(\mathbb{R}^d)$ obtaining the vector in $\Gamma_\mathrm{s}(L^2(\Lambda))$ equal

$$\begin{aligned}
\Theta(T, \omega, \mathbf{q}) &:= \Big(\Phi_{\mathbf{p}_\mathrm{f}} \Big| \Theta(T, \mathbf{p}_\mathrm{i}) \Big) \\
&= -\frac{2\lambda\mathrm{i}}{V}\,\mathrm{e}^{-\mathrm{i}T(H_0 + E + \sigma_\mathrm{f} + \sigma_\mathrm{i})}\,\frac{\sin T(H_0 - E - \omega)}{H_0 - E - \omega} \int\int w(\mathbf{x} - \mathbf{y}) a_\mathbf{x}^* a_\mathbf{x} \Psi\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{y}}\,\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} \\
&= -\frac{2\lambda\mathrm{i}}{V}\,\mathrm{e}^{-\mathrm{i}T(H_0 + E + \sigma_\mathrm{f} + \sigma_\mathrm{i})}\,\frac{\sin T(H_0 - E - \omega)}{H_0 - E - \omega} \hat{w}(\mathbf{q}) N_\mathbf{q} \Psi.
\end{aligned}$$

Note that the number of states in a cube $\mathrm{d}\mathbf{q}_1 \cdots \mathrm{d}\mathbf{q}_d$ equals equals $V(2\pi)^{-d}\mathrm{d}\mathbf{q}_1 \cdots \mathrm{d}\mathbf{q}_d$. Therefore, the scattering crosssection per unit time in the Born approximation is

$$\begin{aligned}
& \frac{1}{2T}\|\Theta(T,\omega,\mathbf{q})\|^2 V(2\pi)^{-d} \\
= \quad & \frac{2\lambda^2}{V^2}|\hat{w}(\mathbf{q})|^2 \left(\Psi \middle| N_{\mathbf{q}}^* \frac{\sin^2 T(H_0 - E - \omega)}{T(H_0 - E - \omega)^2} N_{\mathbf{q}} \Psi \right) V(2\pi)^{-d} \\
\underset{T\to\infty}{\longrightarrow} \quad & (2\pi)^{1-d}\lambda^2 \rho |\hat{w}(\mathbf{q})|^2 S(\omega,\mathbf{q}),
\end{aligned} \tag{H.5}$$

where $\rho = \frac{\langle N \rangle}{V}$ is as usual the density and

$$S(\omega,\mathbf{q}) = \langle N \rangle^{-1}(\Psi|N_{\mathbf{q}}^* \delta(H - E - \omega) N_{\mathbf{q}}\Psi) \tag{H.6}$$

is sometimes called the *van Hove formfactor.*

It is interesting to note that (H.5) depends on the incoming and outgoing data only through the momentum and energy transfer.

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