DOI 10.4171/8ECM/04

Bogoliubov excitation spectrum of Bose gases

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Abstract. We review some rigorous results on the derivation of Bogoliubov excitation spectrum of interacting Bose gases from many-body Schrödinger equations.

1. Introduction

The Bose–Einstein condensation (BEC) has been an important topic in quantum physics for a long time since the first predictions in 1924 [11, 24], and especially after the experimental observations in 1995 [2, 19]. Roughly speaking, BEC is the phenomenon when many bosons occupy a common quantum state at very low temperatures, thus allowing to observe in our macroscopic scales many interesting quantum phenomena such as superfluidity and quantized vortices.

While the pioneer works of Bose and Einstein [11, 24] concern only the *non-interacting* gas, in reality the particles do interact and the rigorous understanding of *interacting* systems remains a very challenging problem in mathematical physics. The theory of interacting Bose gases essentially started in 1947 when Bogoliubov [10] proposed an approximation theory and used it to predict the excitation spectrum of Bose gases. In particular, Bogoliubov's theory gives a satisfactory explanation of Landau's criterion for superfluidity [32]. Since then, there have been several attempts to justify Bogoliubov's theory from first principles, namely from many-body Schrödinger equations, and some rigorous results will be reviewed below.

Heuristically, Bogoliubov's theory based on the key assumption that *the interaction is sufficiently weak*. In this case, the total interaction felt by each particle can be effectively replaced by a one-body mean-field potential, in the spirit of the law of large number in probability theory. This so-called *mean-field approximation* leads to Hartree's theory (or the Gross–Pitaevskii theory) which has been used widely to study the condensate. Moreover, the weak interaction ansatz also allows to treat excited particles by the second-order perturbation method. Consequently, Bogoliubov's theory

2020 Mathematics Subject Classification. 81V73.
Keywords. Bose gases, Bose–Einstein condensation, Bogoliubov's theory.

gives an effective description for the fluctuations around the condensate, as some sort of the central limit theorem.

In this review, we will focus on two specific scaling regimes where the interactions are weak but still play a leading order role.

- The *mean-field regime*: the interaction range is long, but the interaction strength is weak. Thus there are many but weak collisions, which is an ideal situation to apply the mean-field approximation.
- The *Gross–Pitaevskii regime*: the interaction range is short, but the interaction strength is strong. Thus there are few but strong collisions, making the mean-field behavior less obvious.

Although the mean-field and Gross–Pitaevskii regimes correspond to different physical systems, it turns out that Bogoliubov's arguments apply successfully to both cases. In fact, thanks to a series of works by many authors in the last 10 years, the validity of Bogoliubov excitation spectrum has been proved in both regimes. In 2011, Seiringer [55] for the first time justified the Bogoliubov excitation spectrum in the mean-field regime for the homogeneous Bose gas in the torus $\mathbb{T}^3$. Later his result was extended to general trapped systems in $\mathbb{R}^3$ in [30,36]; see also [8,13,21,46,49,52,54] for various extensions. On the other hand, in the Gross–Pitaevskii regime, which is most relevant to the physical setup in [2, 19], the analysis is significantly more challenging since Bogoliubov's theory admits a subtle correction. The correction to Bogoliubov's theory in the Gross–Pitaevskii regime was established by Boccato, Brennecke, Cenatiempo, and Schlein [7] for the homogeneous gas. Very recently, this result was finally extended to general trapped systems in $\mathbb{R}^3$ in [17,50].

In the following, I will explain in detail Bogoliubov's theory and review the results obtained in [36, 50]. I will also discuss some possible extensions and open problems in the end.

2. Bogoliubov's theory

To make the idea transparent, let us start with a trapped system in the mean-field regime. We consider a system of N bosons in $\mathbb{R}^3$ described by the Hamiltonian

$$H_N = \sum_{i=1}^{N} \big(-\Delta_{x_i} + V_{\mathrm{ext}}(x_i) \big) + \frac{1}{N-1} \sum_{1 \le i < j \le N} W(x_i - x_j) \tag{2.1}$$

which acts on the symmetric space $\mathfrak{H}^N = \bigotimes_{\mathrm{sym}}^N L^2(\mathbb{R}^3)$. Here $x_i \in \mathbb{R}^3$ stands for the coordinate of the ith particle (we ignore the spin for simplicity) and $\mathfrak{H}^N$ consists of functions in $L^2((\mathbb{R}^3)^N)$ satisfying

$$\Psi(x_1, \ldots, x_N) = \Psi(x_{\tau(1)}, \ldots, x_{\tau(N)}), \quad \forall \tau \in S_N.$$

We assume that the external potential $V_{\rm ext} : \mathbb{R}^3 \to \mathbb{R}$ satisfies

$$(V_{\rm ext})_- \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3), \quad (V_{\rm ext})_+ \in L^1_{\rm loc}(\mathbb{R}^3), \quad \lim_{|x|\to\infty} V_{\rm ext}(x) = \infty \quad (2.2)$$

and that the interaction potential $W : \mathbb{R}^3 \to \mathbb{R}$ satisfies

$$W^2 \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3). \quad (2.3)$$

Under these conditions, H_N is well defined on the core domain $\bigotimes_{\rm sym}^N C_c^\infty(\mathbb{R}^3)$ and it is bounded from below. Consequently, H_N can be extended to be a self-adjoint operator on $\mathfrak{H}^N$ by Friedrichs' method. The trapping condition $\lim_{|x|\to\infty} V_{\rm ext}(x) = \infty$ ensures that H_N has a compact resolvent, and hence it has eigenvalues

$$\lambda_1(H_N) \le \lambda_2(H_N) \le \cdots, \quad \lim_{j\to\infty} \lambda_j(H_N) = \infty.$$

We are interested in the asymptotic behavior of the eigenvalues of H_N when $N \to \infty$.

In the non-interacting gas, namely $W = 0$, the spectrum of H_N can be computed explicitly from the spectrum of the one-body operator $-\Delta + V_{\rm ext}$ as follows:

$$\sigma(H_N) = \left\{ \sum_{i\ge1} n_i e_i \mid e_i \in \sigma(-\Delta + V_{\rm ext}),\ n_i \in \{0,1,2,\dots\},\ \sum_{i\ge1} n_i = N \right\}.$$

On the other hand, for the interacting gas, namely $W \neq 0$, it is in general impossible to compute the spectrum of H_N when N becomes large, even numerically. Therefore, it is important to derive effective theories, which are less precise (describing only some collective properties of the system) but easier to deal with.

One of the most popular approximation methods used in computational quantum physics and chemistry is the *mean-field approximation*, which was first introduced by Curie and Weiss to describe phase transitions in statistical mechanics. Heuristically, the mean-field theory is based on the assumption that the particles are *independent*, leading to a replacement of the *linear* problem of N particles by a *non-linear* problem of one particle. Mathematically, N independent and identical particles can be described by the Hartree state

$$\Psi(x_1,\dots,x_N) = u^{\otimes N}(x_1,\dots,x_N) = u(x_1)\cdots u(x_N),$$

where u is a normalized function in $L^2(\mathbb{R}^3)$. The energy per particle of the factorized wave function $u^{\otimes N}$ is given by the *Hartree functional*

$$\mathcal{E}_{\rm H}(u) = \int_{\mathbb{R}^3} \left(\left|\nabla u(x)\right|^2 + V_{\rm ext}(x)\left|u(x)\right|^2\right) {\rm d}x + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \left|u(x)\right|^2\left|u(y)\right|^2 W(x-y)\,{\rm d}x\,{\rm d}y.$$

In Hartree's theory, the lowest energy per particle is

$$e_{\mathrm{H}} = \inf_{\|u\|_{L^2(\mathbb{R}^3)}=1} \mathcal{E}_{\mathrm{H}}(u).$$

It is not difficult to show that e_{H} has a minimizer u_0 which is non-negative and solves the self-consistent equation

$$Du_0 = 0, \quad D = -\Delta + V_{\mathrm{ext}} + |u_0|^2 * W - \varepsilon_0, \tag{2.4}$$

where ε_0 is a real constant (it is the Lagrange multiplier associated with the mass constraint $\|u\|_{L^2(\mathbb{R}^3)} = 1$). Thus the mean-field approximation suggests that the ground state energy of H_N in (3.7) satisfies

$$E_N = Ne_{\mathrm{H}} + o(N)_{N\to\infty} \tag{2.5}$$

and that u_0 describes the Bose–Einstein condensate. We refer to [34] and the reviews [33, 53] for rigorous results on the validity of Hartree's theory.

In this review, we are interested in the next order correction to Hartree's theory, which is given by Bogoliubov's theory. We will give below two different heuristic derivations of Bogoliubov's theory: the first is obtained by applying the second-order perturbation method to the Hartree functional, and the second is obtained by manipulating the many-body Hamiltonian in the second quantization language. While the first is shorter and easier to access for a general audience, the second is closer to Bogoliubov's original argument [10] and easier to justify mathematically.

2.1. Bogoliubov's theory from the second-order perturbation

To describe the excited particles, namely the particles outside of the condensate, we can apply the second-order perturbation method to the Hartree functional. More precisely, if u_0 is a Hartree minimizer, then for $v \perp u_0$ we have the Taylor expansion

$$\mathcal{E}_{\mathrm{H}}\left(\frac{u_0 + v}{\sqrt{1 + \|v\|_{L^2}^2}}\right) = e_{\mathrm{H}} + \frac{1}{2}\left\langle \begin{pmatrix} v \\ \bar{v} \end{pmatrix}, \mathcal{E}_{\mathrm{H}}''(u_0) \begin{pmatrix} v \\ \bar{v} \end{pmatrix} \right\rangle + o\left(\|v\|_{H^1(\mathbb{R}^3)}^2\right) \tag{2.6}$$

with the Hessian matrix

$$\mathcal{E}_{\mathrm{H}}''(u_0) = \begin{pmatrix} D + K & K \\ K & D + K \end{pmatrix},$$

where K is the operator on $L^2(\mathbb{R}^3)$ with kernel

$$K(x, y) = u_0(x)u_0(y)w(x - y).$$

Roughly speaking, Bogoliubov's theory suggests that we may lift the Taylor expansion (2.6) to the many-body level, leading to the following refinement of (2.5):

$$\sigma(H_N) = Ne_{\mathrm{H}} + \sigma(\mathbb{H}_{\mathrm{Bog}}) + o(1)_{N\to\infty}, \tag{2.7}$$

where the Bogoliubov Hamiltonian $\mathbb{H}_{\mathrm{Bog}}$ is the *second quantization* of $\frac{1}{2}\mathcal{E}''_{\mathrm{H}}(\varphi)$ that we will introduce later.

Note that we always have $\mathcal{E}''_{\mathrm{H}}(\varphi) \geq 0$ since u_0 is a Hartree minimizer (in particular $D \geq 0$ and u_0 is a ground state of D). Moreover, it is known that if the Hessian matrix is non-degenerate, namely

$$\mathcal{E}''_{\mathrm{H}}(\varphi) \geq \eta > 0 \quad \text{on } \mathfrak{H}_+ \oplus \mathfrak{H}_+ \tag{2.8}$$

with $\mathfrak{H}_+ = \{u_0\}^\perp \subset L^2(\mathbb{R}^3)$ and a constant $\eta > 0$, then it can be diagonalized by a symplectic matrix of the form

$$\mathcal{V} = \begin{pmatrix} \sqrt{1+s^2} & s \\ s & \sqrt{1+s^2} \end{pmatrix}, \quad \mathcal{V}^* \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{V} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.9}$$

namely

$$\mathcal{V}^* \mathcal{E}''_{\mathrm{H}}(\varphi) \mathcal{V} = \begin{pmatrix} E_\infty & 0 \\ 0 & E_\infty \end{pmatrix}, \tag{2.10}$$

where E_∞ is unitarily equivalent to $(D^{1/2}(D+2K)D^{1/2})^{1/2}$. Consequently, up to a constant, the Bogoliubov Hamiltonian $\mathbb{H}_{\mathrm{Bog}}$ is unitarily equivalent to $\mathrm{d}\Gamma(E_\infty)$, the quantization of E_∞ (see (2.14) below). We refer to [20, 48] for general discussions on the diagonalization procedure, in particular for the emergence of the symplectic structure in (2.9). In summary, (2.8) implies that the excitation spectrum of H_N can be described by the spectrum of E_∞ as follows:

$$\begin{aligned} \sigma(H_N) - \lambda_1(H_N) &\approx \sigma\big(\mathrm{d}\Gamma(E_\infty)\big) \\ &= \Big\{ \sum_{i\geq 1} n_i e_i \mid e_i \in \sigma(E_\infty),\ n_i \in \{0,1,\ldots\} \Big\}. \end{aligned} \tag{2.11}$$

2.2. Bogoliubov's theory from the microscopic equation

Now we explain Bogoliubov's theory from the microscopic description of the many-body system, which is closer to the original argument in [10].

Let us recall the Fock space formalism. Let $\mathfrak{K}$ be $L^2(\mathbb{R}^3)$ or a subspace of $L^2(\mathbb{R}^3)$. We define the bosonic Fock space

$$\mathcal{F}(\mathfrak{K}) = \bigoplus_{n=0}^{\infty} \mathfrak{K}^n, \quad \mathfrak{K}^n = \bigotimes_{\mathrm{sym}}^{n} \mathfrak{K}. \tag{2.12}$$

For $g \in \mathfrak{K}$, we define the creation and annihilation operators $a^*(g)$, $a(g)$ on $\mathcal{F}(\mathfrak{K})$ by

$$\big(a^*(g)\Psi\big)(x_1,\dots,x_{n+1}) = \frac{1}{\sqrt{n+1}}\sum_{j=1}^{n+1} g(x_j)\Psi(x_1,\dots,x_{j-1},x_{j+1},\dots,x_{n+1}),$$

$$\big(a(g)\Psi\big)(x_1,\dots,x_{n-1}) = \sqrt{n}\int_{\mathbb{R}^3}\overline{g(x_n)}\Psi(x_1,\dots,x_n)\,\mathrm{d}x_n, \quad \forall\Psi\in\mathfrak{K}^n,\ \forall n.$$

It is also convenient to define the operator-valued distributions

$$a_x^* = \sum_{n=1}^{\infty}\overline{f_n(x)}a^*(f_n), \quad a_x = \sum_{n=1}^{\infty} f_n(x)a(f_n), \quad x\in\mathbb{R}^3,$$

where $\{f_n\}_{n=1}^{\infty}$ is an orthonormal basis of $\mathfrak{K}$ (the definitions of a_x, a_x^* are independent of the choice of the basis). Equivalently, we have

$$a^*(g) = \int_{\mathbb{R}^3} g(x)a_x^*\,\mathrm{d}x, \quad a(g) = \int_{\mathbb{R}^3}\overline{g(x)}a_x\,\mathrm{d}x, \quad \forall g\in\mathfrak{K}.$$

These operators satisfy the canonical commutation relations (CCR)

$$\big[a(g_1),a(g_2)\big] = \big[a^*(g_1),a^*(g_2)\big] = 0, \quad \big[a(g_1),a^*(g_2)\big] = \langle g_1,g_2\rangle, \quad \forall g_1,g_2\in\mathfrak{K},$$
$$[a_x^*,a_y^*] = [a_x,a_y] = 0, \quad [a_x,a_y^*] = \delta(x-y), \quad \forall x,y\in\mathbb{R}^3. \tag{2.13}$$

It turns out that many important operators on Fock space can be expressed in the second quantization form using the creation and annihilation operators. For example, for any one-body self-adjoint operator A we can write its second quantization as

$$\mathrm{d}\Gamma(A) := \bigoplus_{n=0}^{\infty}\Big(\sum_{i=1}^{n} A_{x_i}\Big) = \iint_{\mathbb{R}^3} A(x,y)a_x^*a_y\,\mathrm{d}x\,\mathrm{d}y, \tag{2.14}$$

where $A(x,y)$ is the kernel of A. Similarly, the Hamiltonian in (2.1) can be extended to be an operator on $\mathcal{F}(L^2(\mathbb{R}^3))$ as

$$H_N = \int_{\mathbb{R}^3} a_x^*\big(-\Delta_x + V_{\mathrm{ext}}(x)\big)a_x\,\mathrm{d}x + \frac{1}{2N}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} W(x-y)a_x^*a_y^*a_xa_y\,\mathrm{d}x\,\mathrm{d}y. \tag{2.15}$$

Roughly speaking, Bogoliubov's theory [10] contains three key steps.

Step 1 (c-number substitution). From the assumption on the complete condensation on the Hartree minimizer u_0, namely

$$\big\langle\Psi_N, a^*(u_0)a(u_0)\Psi_N\big\rangle = N + o(N), \tag{2.16}$$

and the commutation relation

$$\big[a(u_0), a^*(u_0)\big] = 1 \ll \big\langle \Psi_N, a^*(u_0)a(u_0)\Psi_N\big\rangle = N_0 \approx N,$$

we see that $a(u_0)$ and $a^*(u_0)$ "mostly commute." Pushing this idea further, we may heuristically think of $a(u_0)$ and $a^*(u_0)$ as the scalar number $N_0^{1/2}$. Put differently, we may factor out the contribution of the condensate as a scalar field as

$$a_x \approx N_0^{1/2} u_0(x) + c_x, \tag{2.17}$$

where a_x, c_x are annihilation operators on $\mathcal{F}(\mathfrak{H})$, $\mathcal{F}(\mathfrak{H}_+)$, respectively, where $\mathfrak{H} = L^2(\mathbb{R}^3)$ and $\mathfrak{H}_+ = \{u_0\}^\perp \subset \mathfrak{H}$. This allows us to focus on the Fock space $\mathcal{F}(\mathfrak{H}_+)$ which corresponds to excited particles.

Step 2 (Quadratic reduction). Inserting (2.17) in (2.15) and expanding to second order, we obtain

$$H_N \approx N e_{\rm H} + \mathbb{H}_{\rm Bog} + o(1)_{N\to\infty}, \tag{2.18}$$

where

$$\mathbb{H}_{\rm Bog} = {\rm d}\Gamma(D) + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} W(x-y)u_0(x)u_0(y)(2c_x^*c_y + c_x^*c_y^* + c_xc_y)\,{\rm d}x\,{\rm d}y. \tag{2.19}$$

Here we have ignored all terms containing more than 2 operators c_x or c_x^* thanks to the BEC (heuristically $c_x \ll N^{1/2} \approx N_0^{1/2}$). Moreover, the terms containing only one operator c_x or c_x^* are canceled due to the Hartree's equation (2.4).

Note that the Bogoliubov Hamiltonian in (2.19) can be rewritten as

$$\mathbb{H}_{\rm Bog} = \int_{\mathbb{R}^3} c_x^*(D+K)_x c_x\,{\rm d}x + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K(x,y)(c_x^*c_y^* + c_xc_y)\,{\rm d}x\,{\rm d}y$$

which is exactly the second quantized version of the Hessian energy

$$\frac{1}{2}\left\langle \begin{pmatrix} v \\ v \end{pmatrix}, \mathcal{E}''_{\rm H}(\varphi)\begin{pmatrix} v \\ v \end{pmatrix}\right\rangle = \int \overline{v(x)}(D+K)v(x)\,{\rm d}x + \frac{1}{2}\iint K(x,y)\big(v(x)v(y) + \overline{v(x)v(y)}\big)\,{\rm d}x\,{\rm d}y$$

via the simple rules $\overline{v(x)} \mapsto a_x^*$, $v(x) \mapsto a_x$.

Step 3 (Diagonalization). The Bogoliubov Hamiltonian $\mathbb{H}_{\rm Bog}$ in (2.18) can be diagonalized by a unitary operator on $\mathcal{F}(\mathfrak{H}_+)$ of the form

$$T = \exp\left(\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\big(k(x,y)c_x^*c_y^* - {\rm h.c.}\big)\,{\rm d}x\,{\rm d}y\right)$$

with an appropriate kernel $k(x,y)$. The actions of T are characterized by

$$T^* c(v) T = c(\sqrt{1+s^2}v) + c^*(sv),$$
$$T^* c^*(v) T = c^*(\sqrt{1+s^2}v) + c(sv), \quad \forall v \in \mathfrak{H}_+,$$

where

$$s = \mathrm{sh}(k) = \frac{e^k - e^{-k}}{2}$$

with k being the operator with kernel $k(x,y)$. If we choose the operator s as in (2.10), then a simple computation using the CCR (2.13) leads to the identity

$$T^* \mathbb{H}_{\mathrm{Bog}} T = \frac{1}{2} Tr_{\mathfrak{H}_+}(E_\infty - D - K) + \mathrm{d}\Gamma(E_\infty). \tag{2.20}$$

Thus from (2.18) we deduce that, up to a unitary transformation,

$$H_N \approx N e_{\mathrm{H}} + \frac{1}{2} Tr_{\mathfrak{H}_+}(E_\infty - D - K) + \mathrm{d}\Gamma(E_\infty) + o(1)_{N\to\infty}, \tag{2.21}$$

which is consistent with the prediction in (2.11) for the excitation spectrum.

3. Validity of Bogoliubov's theory

3.1. The mean-field regime

In this subsection we focus on the mean-field regime, namely we consider the Hamiltonian in (2.1),

$$H_N = \sum_{i=1}^N \big(-\Delta_{x_i} + V_{\mathrm{ext}}(x_i)\big) + \frac{1}{N-1} \sum_{1\le i<j\le N} W(x_i - x_j),$$

with time-independent potentials V_{ext}, W.

From the heuristic discussion in Section 2, we can easily extract two natural conditions which are necessary to justify Bogoliubov's prediction for the excitation spectrum.

- The Hartree minimizer is unique. This is the necessary and sufficient condition to have the complete BEC in (2.16) for low-lying eigenfunctions of H_N; see, e.g., [33, 34, 53].
- The non-degeneracy (2.8) holds true. This condition ensures that the Taylor expansion in (2.6) makes sense, namely the Hessian dominates the error term, and that the Bogoliubov Hamiltonian in (2.19) is bounded from below and diagonalizable; see [20, 48].

In a joint work with M. Lewin, S. Serfaty, and J. P. Solovej [36], we proved that Bogoliubov's prediction is indeed correct under those general conditions on the Hartree minimizer. More precisely, we have the following theorem.

Theorem 3.1 (Validity of Bogoliubov excitation spectrum [36]). *Consider the Hamiltonian H_N in (2.1), where $V_{\rm ext}$ and W satisfy (2.2) and (2.3). Assume that the Hartree minimizer u_0 is unique and non-degenerate. Then for every $j \in \mathbb{N}$, the jth eigenvalue of H_N satisfies*

$$\lim_{N\to\infty} \big(\lambda_j(H_N) - Ne_{\rm H}\big) = \lambda_j(\mathbb{H}_{\rm Bog}),$$

where the Bogoliubov Hamiltonian is an operator on $\mathcal{F}(\mathfrak{H}_+)$ defined in (2.19).

The result in [36] holds in a more general setting; in particular, it holds in all dimensions and the external potential $V_{\rm ext}$ may vanish at infinity which is relevant to unconfined systems. In the later case, some particles may escape to infinity and we have to add the assumption that any minimizing sequence of the Hartree functional is pre-compact in $L^2(\mathbb{R}^3)$, which is the necessary and sufficient condition for the complete BEC to hold (see [34]).

Our result in [36] was inspired by the pioneer works of Seiringer [55] and Grech and Seiringer [30] who have for the first time derived the Bogoliubov excitation spectrum for a class of trapped bosons in the mean-field model. In [30,55], the interaction potential W is assumed to be bounded and of positive type, namely its Fourier transform satisfies

$$0 \le \widehat{W} \in L^1(\mathbb{R}^3).$$

Under this condition, we have

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \overline{f(x)} f(y) W(x-y)\,\mathrm{d}x\,\mathrm{d}y = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big|\hat{f}(k)\big|^2 \widehat{W}(k)\,\mathrm{d}k \ge 0. \qquad (3.1)$$

Therefore, the uniqueness of the Hartree minimizer is an easy consequence of the convexity of $|u|^2 \mapsto \mathcal{E}_{\rm H}(u)$ (the convexity of the kinetic part follows from the diamagnetic inequality $|\nabla u(x)| \ge |\nabla |u|(x)|$). Moreover, (3.1) also implies that the operator K with kernel $u_0(x)u_0(y)W(x-y)$ is a positive operator, and hence the non-degeneracy condition (2.8) holds true.

Note that thanks to (2.20), the spectrum of $\mathbb{H}_{\rm Bog}$ is known explicitly in terms of the spectrum of the one-body operator E_∞ given in (2.11). For the *homogeneous gas* studied in [55], when particles are confined on the torus $[0, L]^3$ with periodic boundary condition and $V_{\rm ext} = 0$, the eigenvalues of E_∞ are simply given by

$$e_p = \big(|p|^4 + 2|p|^2 \widehat{W}(p)\big)^{1/2}, \quad p \in (2\pi/L)\mathbb{Z}^3 \backslash \{0\}.$$

As already mentioned by Bogoliubov [10], the fact that the elementary excitation e_p behaves linearly for small $|p|$ corresponds to Landau's criterion for superfluidity [32]. More precisely, it implies the wedge-like shape of the joint spectrum of the Hamiltonian momentum, which in particular guarantees that adding a drop with a small velocity will not change the ground state of the system, namely the drop can move without friction. Strictly speaking, the mean-field regime discussed in this subsection corresponds to the choice $L \sim 1$ and $|p|$ is not very small. However, the same picture holds true in the large volume limit $L = L_N \to \infty$; see [21] for rigorous results (the results in [7, 8], up to a suitably scaling argument, are also relevant to the large volume limit).

Ingredients of the proof. Now let us explain the main ideas of the proof in [36]. Our important tool is an *excitation operator* which implements Bogoliubov's c-number substitution. Thanks to the isomorphism of Fock spaces

$$\mathcal{F}\big(L^2(\mathbb{R}^3)\big) = \mathcal{F}\big(\operatorname{Span}(u_0) \oplus \{u_0\}^\perp\big) \approx \mathcal{F}\big(\operatorname{Span}(u_0)\big) \otimes_s \mathcal{F}(\mathfrak{H}_+)$$

we can decompose any function $\Psi_N \in \mathfrak{H}^N$ uniquely as

$$\Psi_N = u_0^{\otimes N}\xi_0 + u_0^{\otimes N-1} \otimes_s \xi_1 + u_0^{\otimes N-2} \otimes_s \xi_2 + \cdots + \xi_N$$

with $\xi_k \in \mathfrak{H}_+^k$. Recall that for two functions $\Psi_k \in \mathfrak{H}^k$ and $\Psi_\ell \in \mathfrak{H}^\ell$, we define the symmetric tensor product by

$$\begin{aligned}\Psi_k \otimes_s \Psi_\ell(x_1, \dots, x_{k+\ell}) \\ = \frac{1}{\sqrt{k!\ell!(k+\ell)!}} \sum_{\tau \in S_N} \Psi_k(x_{\tau(1)}, \dots, x_{\tau(k)})\Psi_\ell(x_{\tau(k+1)}, \dots, x_{\tau(k+\ell)}).\end{aligned}$$

As proved in [36], the operator

$$U : \Psi_N \to (\xi_0, \xi_1, \dots, \xi_N) \tag{3.2}$$

is a unitary transformation from $\mathfrak{H}^N$ to the truncated Fock space

$$\mathcal{F}^{\leq N}(\mathfrak{H}_+) = \mathbf{1}^{\mathcal{N}_+ \leq N}\mathcal{F}(\mathfrak{H}_+),$$

where $\mathcal{N}_+ = d\Gamma(\mathbf{1}_{\mathfrak{H}_+})$ is the number operator on the excited Fock space $\mathcal{F}(\mathfrak{H}_+)$. The operator U essentially maps $a(u_0)$ and $a^*(u_0)$ to $\sqrt{N - \mathcal{N}_+}$, namely

$$a_x \mapsto \sqrt{N - \mathcal{N}_+} u_0(x) + c_x,$$

where c_x is the annihilation operator on $\mathcal{F}(\mathfrak{H}_+)$. More precisely, we have on $\mathcal{F}^{\leq N}(\mathfrak{H}_+)$

$$U H_N U^* = \mathbf{1}^{\mathcal{N} \leq N}\Big(\sum_{i=0}^{4} \mathcal{L}_i\Big)\mathbf{1}^{\mathcal{N} \leq N}, \tag{3.3}$$

where

$$\mathcal{L}_0 = Ne_{\mathrm{H}} + \frac{\mathcal{N}_+(\mathcal{N}_+ + 1)}{2N}\Big(\int |u_0|^2\big(W * |u_0|^2\big)\Big),$$

$$\mathcal{L}_1 = \sqrt{N - \mathcal{N}_+}\int \big(\big(-\Delta + V_{\mathrm{ext}} + |u_0|^2 * W\big)u_0\big)(x)c_x\,\mathrm{d}x + \mathrm{h.c.}$$
$$+ \frac{\mathcal{N}_+\sqrt{N - \mathcal{N}_+}}{N-1}\int \big(\big(|u_0|^2 * W\big)u_0\big)(x)c_x\,\mathrm{d}x + \mathrm{h.c.},$$

$$\mathcal{L}_2 = \int c_x^*(D+K)_x c_x\,\mathrm{d}x + \frac{1-\mathcal{N}_+}{N-1}\int c_x^*\big(|u_0|^2 * W + K\big)_x c_x\,\mathrm{d}x$$
$$+ \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+ - 1)}}{2(N-1)}\iint K(x,y)c_x c_y\,\mathrm{d}x\,\mathrm{d}y + \mathrm{h.c.},$$

$$\mathcal{L}_3 = \frac{\sqrt{N-\mathcal{N}_+}}{N-1}\iint W(x-y)\varphi(x)c_y^* c_x c_y\,\mathrm{d}x\,\mathrm{d}y + \mathrm{h.c.},$$

$$\mathcal{L}_4 = \frac{1}{N-1}\iint W(x-y)c_x^* c_y^* c_x c_y\,\mathrm{d}x\,\mathrm{d}y.$$

By formally taking the limit $N \to \infty$, we obtain immediately the desired convergence

$$UH_NU^* - Ne_{\mathrm{H}} \to \mathbb{H}_{\mathrm{Bog}}. \tag{3.4}$$

Rigorously, we proved in [36, Proposition 5.1] that for every $1 \le M \le N$,

$$\pm \mathbf{1}^{\mathcal{N}_+ \le M}(UH_NU^* - Ne_{\mathrm{H}} - \mathbb{H}_{\mathrm{Bog}})\mathbf{1}^{\mathcal{N}_+ \le M} \le C\sqrt{\frac{M}{N}}(\mathbb{H}_{\mathrm{Bog}} + C) \tag{3.5}$$

as quadratic forms on $\mathcal{F}^{\le M}(\mathfrak{H}_+)$. This justifies the convergence (3.4) in the sectors of *low excitations*, namely $\mathcal{N}_+ \ll N$. The contribution of the sectors of *high excitations*, namely $\mathcal{N}_+ \sim N$, is negligible thanks to the complete BEC (2.16). Using (3.5), we can derive the convergence of quadratic forms in (3.5), which in turns implies the convergence of eigenvalues by the min-max principle.

As a byproduct of our method, we also obtain the information for eigenfunctions.

Theorem 3.2 (Norm approximation for eigenfunctions [36]). *Under the same conditions in Theorem 3.1, the ground state Ψ_N of H_N is simple and satisfies*

$$\lim_{N\to\infty} \|U\Psi_N - \Phi\|_{\mathcal{F}(\mathfrak{H}_+)} = 0, \tag{3.6}$$

where $\Phi \in \mathcal{F}(\mathfrak{H}_+)$ is the unique ground state of the Bogoliubov Hamiltonian $\mathbb{H}_{\mathrm{Bog}}$. A similar convergence holds for the higher eigenfunctions (possibly up to subsequences of $N \to \infty$ in case of degenerate eigenvalues).

The norm approximation (3.6) is much stronger than the complete BEC (2.16). In fact, while (2.16) describes a macroscopic property, (3.6) really contains microscopic information: changing the behavior of a single particle can change the many-body state in norm to the leading order. In particular, (3.6) implies that in the non-interacting case ($W \not\equiv 0$), Ψ_N is *never* close to $u_0^{\otimes N}$ in norm, namely the fluctuations around the Hartree state $u_0^{\otimes N}$ are nontrivial.

3.2. The Gross–Pitaevskii regime

In this subsection, we consider the N-body Hamiltonian

$$H_N = \sum_{i=1}^{N} \big(-\Delta_{x_i} + V_{\mathrm{ext}}(x_i) \big) + \sum_{1 \le i < j \le N} N^2 V\big(N(x_i - x_j) \big) \tag{3.7}$$

on $\mathfrak{H}^N = \bigotimes_{\mathrm{sym}}^N L^2(\mathbb{R}^3)$ with time-independent potentials V_{ext}, V. For simplicity, we assume that the external and interaction potentials satisfy

$$0 \le V_{\mathrm{ext}}(x) \le C e^{C|x|} \text{ for some constant } C > 0, \qquad \lim_{|x| \to \infty} V_{\mathrm{ext}}(x) = \infty, \tag{3.8}$$

$$0 \le V \in L^1(\mathbb{R}^3), \qquad V \text{ is radially symmetric and compactly supported.} \tag{3.9}$$

In this so-called Gross–Pitaevskii regime, the system is very dilute and the strong correlation between particles at short distances leads to a subtle correction to the leading order which is captured by the *scattering length*

$$8\pi \mathfrak{a}_0 = \inf \left\{ \int_{\mathbb{R}^3} \big(2|\nabla f(x)|^2 + V(x)|f(x)|^2 \big)\, \mathrm{d}x, \ \lim_{|x| \to \infty} f(x) = 1 \right\}. \tag{3.10}$$

More precisely, the Hartree functional has to be replaced by the *Gross–Pitaevskii functional*

$$\mathcal{E}_{\mathrm{GP}}(u) = \int_{\mathbb{R}^3} \big(|\nabla u(x)|^2 + V_{\mathrm{ext}}(x)|u(x)|^2 + 4\pi \mathfrak{a}_0 |u(x)|^4 \big)\, \mathrm{d}x. \tag{3.11}$$

Note that by simply restricting to the Hartree states $u^{\otimes N}$ and using $N^3 V(N\cdot) \approx \widehat{V}(0)\delta_0$, we would obtain a *wrong* functional with $8\pi\mathfrak{a}_0$ replaced by its first Born approximation $\widehat{V}(0)$. It is not difficult to prove that the Gross–Pitaevskii functional has a unique normalized minimizer φ which is positive and exponentially decay (see [39]).

In [39], Lieb, Seiringer, and Yngvason proved that the ground state energy of H_N in (3.7) satisfies

$$\lim_{N \to \infty} \frac{\lambda_1(H_N)}{N} = \inf_{\|u\|_{L^2(\mathbb{R}^3)} = 1} \mathcal{E}_{\mathrm{GP}}(u). \tag{3.12}$$

Later, in [37,38], Lieb and Seiringer proved that if Ψ_N is an approximate ground state, namely $\langle \Psi_N, H_N \Psi_N \rangle = \lambda_1(H_N) + o(N)$, then the complete BEC on the Gross–Pitaevskii minimizer φ holds:

$$\big\langle \Psi_N, a^*(\varphi) a(\varphi) \Psi_N \big\rangle = N + o(N). \tag{3.13}$$

Recently, the BEC with *optimal rate*

$$\big\langle \Psi_N, a^*(\varphi) a(\varphi) \Psi_N \big\rangle = N + O(1) \tag{3.14}$$

was obtained in [6, 9, 31] (the homogeneous case) and [18, 47] (the general trapped case).

Since there are only finitely many excited particles due to (3.14), it is still reasonable to predict the excitation spectrum by Bogoliubov's approximation. A straightforward application of the heuristic arguments in Section 2 predicts that the elementary excitations are eigenvalues of the one-body operator

$$\big(D^{1/2}\big(D + 2\widehat{V}(0)\varphi^2\big) D^{1/2}\big)^{1/2},$$

where D is the mean-field operator associated with the Gross–Pitaevskii equation,

$$D\varphi = 0, \quad D = -\Delta + V_{\text{ext}} + 8\pi \mathfrak{a}_0 - \varepsilon_0.$$

However, as mentioned already by Bogoliubov [10] (which goes back to a remark of Landau), the number $\widehat{V}(0)$ should be replaced by the scattering length $8\pi\mathfrak{a}_0$, similarly to the leading order correction. Therefore, to put Bogoliubov's theory in a good use, after the three steps written in Section 2.2, we need an important modification.

Step 4 (Landau's correction). $\widehat{V}(0)$ should be replaced by $8\pi\mathfrak{a}_0$ everywhere, with $\mathfrak{a}_0$ the scattering length of V.

It is Step 4 that makes the implementation of Bogoliubov's arguments in the Gross–Pitaevskii regime much more challenging than that of the mean-field regime.

In [7], Boccato, Brennecke, Cenatiempo, and Schlein solved this problem for the homogeneous gas. Recently, in a joint work with A. Triay [50], we extended the result for general trapped systems. We have the following theorem.

Theorem 3.3 (Bogoliubov's theory in the Gross–Pitaevskii regime [50]). *Consider the Hamiltonian H_N in (3.7). Let $\lambda_1(H_N)$ be the ground state energy of the Hamiltonian H_N in (3.7). Then the spectrum of $H_N - \lambda_1(H_N)$ below an energy $\Lambda \in [1, N^{1/12}]$ is equal to finite sums of the form*

$$\sum_{i \ge 1} n_i e_i + \mathcal{O}(\Lambda^3 N^{-1/12}), \quad n_i \in \{0, 1, 2, \dots\},$$

where $\{e_i\}_{i=1}^\infty$ are the positive eigenvalues of $(D^{1/2}(D + 16\pi\mathfrak{a}_0\varphi^2) D^{1/2})^{1/2}$.

Independently to us, a result similar to Theorem 3.3 was obtained by Brennecke, Schlein, and Schraven in [17]. While our overall approach is similar to that of [7, 17], the detailed implementations are different. In fact, in [50] we introduced several conceptual simplifications and generalizations, which could be helpful for the study of dilute gases in the future. Let us explain some key ideas below.

Ingredients of the proof. Our proof is based on the rigorous approximation

$$T_2^* T_c^* T_1^* U H_N U^* T_1 T_c T_2 \approx \lambda_1(H_N) + \mathrm{d}\Gamma(E_\infty) + o(1)_{N\to\infty} \tag{3.15}$$

on the excited Fock space $\mathcal{F}_+ = \mathcal{F}(\mathfrak{H}_+)$ with $\mathfrak{H}_+ = \{\varphi\}^\perp = QL^2(\mathbb{R}^3)$ with $Q = 1 - |\varphi\rangle\langle\varphi|$.

Here U is the same transformation in (3.2), which factors out the condensation described by the Gross–Pitaevskii minimizer u_0. Consequently, the excited particles are captured by the Hamiltonian in (3.3). Unlike the mean-field regime where $\mathcal{L}_3$ and $\mathcal{L}_4$ are of order $o(1)$, in the Gross–Pitaevskii regime $L_4 \sim N$ and $L_3 \sim O(1)$. Therefore, these terms have to be renormalized by the unitary transformations T_1 and T_c, respectively. After that, we obtain a quadratic Hamiltonian which can be diagonalized by the final unitary transformation T_2.

To define the quadratic transformation T_1, we need to capture the correlation structure of particles. Let $0 \le f \le 1$ be the scattering solution

$$-2\Delta f + Vf = 0 \quad \text{in } \mathbb{R}^3, \qquad \lim_{|x|\to\infty} f(x) = 1. \tag{3.16}$$

We write $\omega = 1 - f$ and for every $0 < \ell \ll 1$ introduce the truncated functions

$$\omega_{\ell,N}(x) = \chi(x/\ell)\omega(Nx), \quad \varepsilon_{\ell,N} = 2\Delta\big(\omega_{\ell,N}(x) - \omega(Nx)\big), \tag{3.17}$$

where $0 \le \chi \le 1$ is a smooth function satisfying $\chi(t) = 1$ if $|x| \le 1/2$ and $\chi(x) = 0$ if $|x| \ge 1$. By choosing T_1 such that

$$T_1^* a^*(g) T_1 = a^*(\sqrt{1 + s_1^2}\, g) + a(s_1 g), \quad \forall g \in \mathfrak{H}, \tag{3.18}$$

where

$$s_1 = Q^{\otimes 2}\tilde{s}_1 \in \mathfrak{H}_+^2, \quad \tilde{s}_1(x,y) = -N\omega_{\ell,N}(x-y)\varphi(x)\varphi(y),$$

we can replace the short range potential $V(N(x-y))$ in $\mathcal{L}_2$ by the longer range potential $\varepsilon_{\ell,N}(x-y)$. Note that $\varepsilon_{\ell,N}$ is supported in $\{\ell/2 \le |x| \le \ell\}$ and

$$N^3 \int_{\mathbb{R}^3} \varepsilon_{\ell,N} = 8\pi\mathfrak{a}_0. \tag{3.19}$$

When ℓ grows slowly, we are essentially placed in the mean-field regime.

The idea of renormalizing the short-range potential by a Bogoliubov transformation was introduced by Benedikter, de Oliveira, and Schlein [4] to derive the Gross–Pitaevskii dynamics on Fock space. In [16], Brennecke and Schlein adapted the approach in [4] to study the quantum dynamics on $\mathfrak{H}^N$, where they used a generalized Bogoliubov transformation on $\mathcal{F}_+^{\le N}$ of the form

$$\exp\left(\frac{1}{2}\iint \mathfrak{K}_1(x,y) b_x^* b_y^* \,\mathrm{d}x\,\mathrm{d}y - \text{h.c.}\right) \quad \text{with } b_x = \sqrt{1-\mathcal{N}/N}\,a_x. \tag{3.20}$$

The transformation (3.20) has been also an essential tool in the study of the spectral problem in a series of papers [6–9, 17, 18]. Our choice of T_1 in (3.18) is different from (3.20) in three aspects.

- First, the operator b_x in (3.20) is not an exact annihilation operator, and hence $\widetilde{T}_1$ only satisfies an approximate form of (3.18). Here our T_1 is a proper Bogoliubov transformation and the exact formula (3.18) simplifies several computations.
- Second, the truncated scattering solution in [4, 16] is defined using Neumann boundary condition on $|x| = \ell N$. Here our choice of $\omega_{\ell,N}$ in (3.17) is simpler and works for a larger class of potentials.
- Third, and most importantly, we take $\ell \ll 1$ instead of $\ell \sim 1$ as in [4, 7, 16]. Thus T_1 renormalizes $\mathcal{L}_2$ efficiently but and leaves the cubic terms $\mathcal{L}_3$ invariant.

To remove the cubic term $\mathcal{L}_3$, we introduce a cubic transformation of the form

$$T_c = e^S, \quad S = \theta_M \iint k_c(x,y,y') a_x^* a_y^* a_y \,\mathrm{d}x\,\mathrm{d}y - \text{h.c.},$$

where $\theta_M \approx \mathbf{1}(\mathcal{N} \le M)$ and $k_c(x,y,y')$ is the kernel of the operator $k_c : \mathfrak{H} \to \mathfrak{H}^2$ defined by

$$k_c = Q^{\otimes 2}\tilde{k}_c Q, \quad \tilde{k}_c(x,y,y') = -N^{1/2}\varphi(x)\omega_{\ell,N}(x-y)\delta_{y,y'}$$

with $\tilde{k}_c(x,y,y')$ the kernel of the operator $k_c : \mathfrak{H} \to \mathfrak{H}^2$. The projections $Q : \mathfrak{H} \to \mathfrak{H}_+$ and $Q^{\otimes 2} : \mathfrak{H}^2 \to \mathfrak{H}_+^2$ ensure that $k_c : \mathfrak{H}_+ \to \mathfrak{H}_+^2$, namely the cubic kernel S acts only on excited particles. The cut-off parameter $1 \ll M \ll N$ in θ_M allows us to control the number of excitations. Consequently, we have the simple expansion

$$T_c^* A T_c \approx A - [S, A] + \frac{1}{2}\big[S, [S, A]\big]$$

and the above choice of S comes from the cancelation

$$\mathcal{L}_3 - \big[S, \mathrm{d}\Gamma(-\Delta) + \mathcal{L}_4\big] \approx 0.$$

Here our cubic transformation is slightly simpler than that of [7] since we did not change $\mathcal{L}_3$ in the previous step. The idea of using a cubic generator goes back to the work of Yau and Yin [56] on the Lee–Huang–Yang formula in the thermodynamic limit. The choice $\ell \ll 1$ is again very helpful to separate high and low momenta.

Finally, we end up with the quadratic Hamiltonian

$$\mathrm{d}\Gamma(D) + \frac{1}{2}\int N^3 \varepsilon_{\ell,N}(x-y)\varphi(x)\varphi(y)(2a_x^* a_y + a_x^* a_y^* + a_x a_y)\,\mathrm{d}x\,\mathrm{d}y$$

which can be diagonalized similarly as in the mean-field regime. We find that

$$T_2^* T_c^* T_1^* \mathcal{H} T_1 T_c T_2 \approx \mathrm{const} + \mathrm{d}\Gamma(E), \tag{3.21}$$

where

$$E = \big(D^{1/2}(D+2K)D^{1/2}\big)^{1/2}, \quad K = Q\widetilde{K}Q,\ \widetilde{K}(x,y) = \varphi(x)N^3\varepsilon_{\ell,N}(x-y)\varphi(y).$$

Since $\ell \ll 1$, we have $N^3\varepsilon_{N,\ell} \to 8\pi\delta_0$, which implies that $E \to E_\infty$ in an appropriate sense. This completes the overview of our proof of Theorem 3.3.

4. Further results and open problems

Excitation spectrum. In the mean-field regime, the validity of Bogoliubov's theory for the ground state energy and the excitation spectrum were extended in various directions, including the large volume setting [21], multiple-condensations [49, 54], mixture of Bose gases [41], and higher-order expansions [13, 42, 46, 52]. The intermediate regime between the mean-field and the Gross–Pitaevskii regime was studied in [8]. The regime beyond the Gross–Pitaevskii was studied in [14] (see also [1, 27] for results on the BEC). It is an interesting open problem to extend the results in the Gross–Pitaevskii regime (or beyond) to trapped systems in bounded domains with Neumann or Dirichlet boundary conditions, since this will have interesting implications to systems in the thermodynamic limit.

Quantum dynamics. In the mean-field regime, the method in [36] was developed in [35] to derive the norm approximation for the many-body Schrödinger dynamics. Higher-order expansions in the mean-field regime were also obtained in [12]. The validity of Bogoliubov's theory for the quantum dynamics with singular interaction potentials of the form $N^{3\beta}W(N^\beta x)$ with $0<\beta<1$ was obtained in [15, 43–45]. When $\beta = 1$, the Gross–Pitaevskii dynamics was derived in [25, 26], but the justification of Bogoliubov's theory for the dynamics remains open. We refer to the reviews [5, 51] for further discussions on the dynamical problem.

Positive temperatures. As discussed in Section 3, Bogoliubov's theory holds true for eigenvalues belonging to an interval of order 1 above $\lambda_1(H_N)$. This implies the validity of Bogoliubov's theory for the free energy of a temperature of order 1; see, e.g., [36, Theorem 2.3] for an explicit statement. It is an open problem to extend the analysis to higher temperatures. For the homogeneous gas in a unit torus, the critical temperature where we see the BEC phase transition is of order $N^{2/3}$. In this case, the validity of the Gross–Pitaevskii theory has been understood [22], but the validity of Bogoliubov's theory remains unknown.

Thermodynamic limit. In the thermodynamic limit, Bogoliubov's theory is consistent with the Lee–Huang–Yang formula on the ground state energy of dilute Bose gases. In this problem, the leading order behavior is already difficult: the upper bound was proved in 1957 [23] but the lower bound was obtained only some 40 years later [40]. The second order, which requires a correction to Bogoliubov's theory similar to that in the Gross–Pitaevskii regime, was proved recently in [3, 56] (upper bound) and [28, 29] (lower bound). While the second-order lower bound in [29] covers a large class of interaction potentials, including the hard core case, extending this universality to the second-order upper bound remains an open problem. The excitation spectrum seems to be completely out of reach by current techniques; a simple reason is that the existence of the BEC in the thermodynamic limit remains a major open problem in mathematical physics.

Acknowledgments. I would like to thank Mathieu Lewin, Sylvia Serfaty, Jan Philip Solovej, and Arnaud Triay for the collaborations leading to the results reviewed here. I thank Christian Brennecke, Søren Fournais, Christian Hainzl, Marcin Napiórkowski, Benjamin Schlein, and Robert Seiringer for helpful discussions on various aspects of Bogoliubov's theory.

Funding. This research supported in part by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy (EXC-2111-390814868).

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