The Excitation Spectrum of Weakly Interacting Bosons

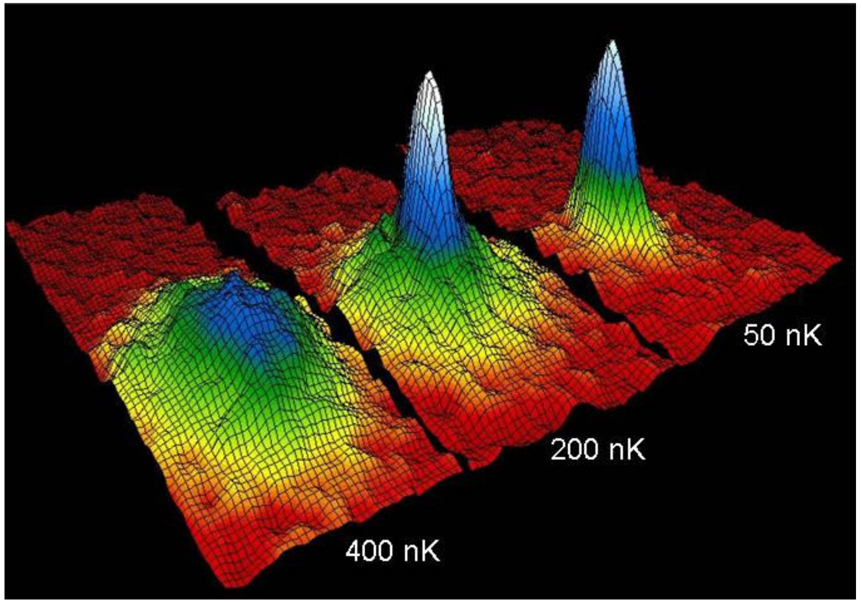
Robert Seiringer
IST Austria

Applications of Bogoliubov Theory

Online Summer School, June 19, 2020

Introduction

First realization of **Bose-Einstein Condensation** (BEC) in cold atomic gases in 1995:



In these experiments, a large number of (bosonic) atoms is confined to a trap and cooled to very low temperatures. Below a **critical temperature** condensation of a large fraction of particles into the same one-particle state occurs.

Interesting **quantum phenomena** arise, like the appearance of quantized vortices and superfluidity. The latter is related to the low-energy **excitation spectrum** of the system.

BEC was predicted by Einstein in 1924 from considerations of the **non-interacting** Bose gas. The presence of particle interactions represents a major difficulty for a rigorous derivation of this phenomenon.

The Bose Gas: A Quantum Many-Body Problem

Quantum-mechanical description in terms of the **Hamiltonian** for a gas of N bosons in a trap potential $V(x)$, interacting via a pair-potential $v(x)$. In appropriate units,

$$H_N = \sum_{i=1}^{N} \big(-\Delta_i + V(x_i) \big) + \sum_{1 \leq i < j \leq N} v(x_i - x_j)$$

The kinetic energy is described by the Δ, the Laplacian on $\mathbb{R}^3$.

As appropriate for **bosons**, H acts on **permutation-symmetric** wave functions $\Psi(x_1, \ldots, x_N)$ in $\bigotimes^N L^2(\mathbb{R}^3)$.

The interaction v is assumed to be **repulsive** and of **short range**.

We will be interested in the **excitation spectrum**, i.e., the eigenvalues of H near the ground state energy $E_0(N) = \inf \operatorname{spec} H_N$.

Weak Interactions

To describe a regime of weak interactions, one can consider the **mean-field** or **Hartree** scaling, where one takes

$$H_N = \sum_{i=1}^{N} \left(-\Delta_i + V(x_i) \right) + \frac{1}{N} \sum_{1\le i<j\le N} v(x_i - x_j)$$

In this case, kinetic, trapping and interaction energies are of the same order for large N. In this limit, one has

$$\lim_{N\to\infty} \frac{E_0(N)}{N} = E^{\mathrm{H}} = \min_{\phi} \mathcal{E}^{\mathrm{H}}(\phi)$$

where

$$\mathcal{E}^{\mathrm{H}}(\phi) = \int_{\mathbb{R}^3} \left(|\nabla \phi(x)|^2 + V(x)|\phi(x)|^2 \right) dx + \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |\phi(x)|^2 v(x-y) |\phi(y)|^2 dx\, dy$$

In addition, there is **complete Bose–Einstein condensation** in the ground state, with condensate wave function giving by the minimizer of the Hartree functional, which will be denoted by ϕ_0 (and will be assumed to be unique).

The Bogoliubov Approximation

In the language of second quantization, H_N equals

$$\int_{\mathbb{R}^3} \left(\nabla a^\dagger(x) \nabla a(x) + V(x) a^\dagger(x) a(x)\right) dx + \frac{1}{2N} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} a^\dagger(x) a^\dagger(y) v(x-y) a(y) a(x) dx dy$$

The **Bogoliubov approximation** consists of writing $a(x) = \sqrt{N}\phi_0(x) + b(x)$ and dropping all terms higher than quadratic in $b(x)$.

The zeroth order term is simply $\mathcal{E}^H(\phi_0) = E^{\mathrm{H}}$. The resulting quadratic Hamiltonian reads

$$H^{\mathrm{Bog}} = \int_{\mathbb{R}^3} \left(\nabla b^\dagger(x) \nabla b(x) + V(x) b^\dagger(x) b(x) + |\phi_0|^2 * v(x) b^\dagger(x) b(x)\right) dx$$
$$+ \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} w(x,y) \left(2 b^\dagger(x) b(y) + b^\dagger(x) b^\dagger(y) + b(x) b(y)\right) dx dy$$

where $w(x,y) = \phi_0(x) v(x-y) \phi_0(y)$, and $*$ denotes convolution.

Bogoliubov Transformation

The quadratic operator H^{Bog} can be diagonalized via a **Bogoliubov transformation**: Let

$$K = -\Delta + V(x) + |\phi_0|^2 * v(x) - \varepsilon_0 \quad , \quad \varepsilon_0 = E^{\mathrm{H}} + \frac{1}{2}\int_{\mathbb{R}^3\times\mathbb{R}^3} |\phi_0(x)|^2 v(x-y)|\phi_0(y)|^2 dxdy$$

and

$$E = \left(K^{1/2}\,(K+2w)\,K^{1/2}\right)^{1/2}$$

Then

$$UH^{\mathrm{Bog}}U^\dagger = E^{\mathrm{Bog}} + \sum_i e_i a_i^\dagger a_i$$

where $e_i > 0$ are the (non-zero) eigenvalues of E, and the a_i are suitable linear combinations of $\int f(x)b^\dagger(x)$ and $\int f(x)b(x)dx$, respectively, with $\int \phi_0(x)f(x)dx = 0$.

In particular, the **excitation spectrum** of H^{Bog} is of the form

$$\sum_i e_i n_i \qquad \text{with } n_i \in \mathbb{N}.$$

Main Results

THEOREM 1 (Grech, S, 2013). *The* **ground state energy** $E_0(N)$ *of* H_N *equals*

$$\boxed{E_0(N) = NE^H + E^{\rm Bog} + O(N^{-1/2})}$$

with

$$E^{\rm Bog} = \frac{1}{2}\,\mathrm{Tr}\,(E - K - w)$$

Moreover, the **excitation spectrum** *of* $H_N - E_0(N)$ *below an energy* ξ *is equal to*

$$\boxed{\sum_i e_i n_i + O\left(\xi^{3/2} N^{-1/2}\right)}$$

where $e_i > 0$ *are the eigenvalues of* E*, and* $n_i \in \{0, 1, 2, \dots\}$ *for all* i.

The proof consists of constructing a unitary operator U that makes $UH_NU^\dagger$ close to the operator $NE^{\rm H} + E^{\rm Bog} + \sum_i e_i a_i^\dagger a_i$. In particular, the **excited eigenfunctions** can be obtained by acting with products of $Ua_i^\dagger a_0 U^\dagger$ on the ground state!

Eigenvalues of $\boldsymbol{E}$

The emergence of the effective operator E can also be understood as follows. One considers the **time-dependent Hartree equation**

$$i\partial_t \phi(x,t) = (-\Delta + V(x) + v * |\phi(x,t)|^2)\phi(x,t)$$

and looks for solutions of the form

$$\phi(x,t) = e^{-i\varepsilon_0 t}(\phi_0(x) + u(x)\, e^{-i\omega t} + \overline{y(x)}\, e^{i\omega t})$$

for some $\omega > 0$. Expanding to first order in u and y leads to the **Bogoliubov–de-Gennes equations**

$$\begin{pmatrix} K+w & w \\ -w & -(K+w) \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \omega \begin{pmatrix} u \\ y \end{pmatrix}.$$

The positive values which can be assumed by ω are then interpreted as excitation energies. This is in agreement with our result: the values for ω obtained this way are precisely the eigenvalues of E.

The Translation-Invariant Case

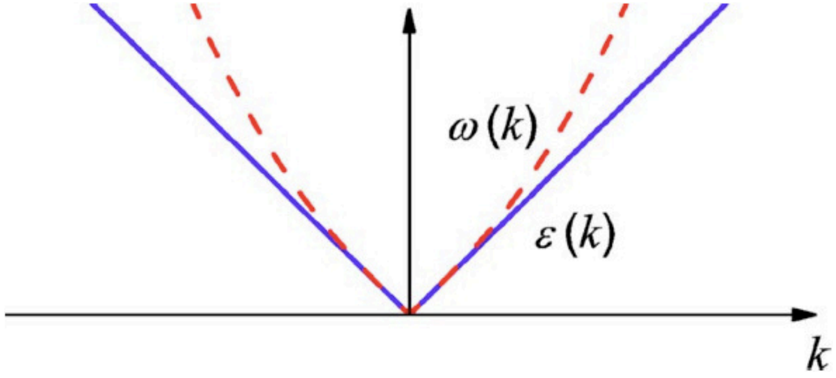
In the absence of a trap ($V(x) = 0$, and the particles confined to a torus), H_N commutes with the **total momentum** $P = -i\sum_{j=1}^{N} \nabla_j$ and hence one can look at their **joint spectrum**. Of particular relevance is the infimum

$$E_q(N) = \inf \operatorname{spec} H_N \restriction_{P=q}$$

The operator E is then diagonal in momentum space, with eigenvalues

$$e_p = |p|\sqrt{2\widehat{v}(p) + |p|^2}$$

In particular, for interacting systems one obtains a **linear** behavior of $E_q(N) - E_0(N)$ for small q.



The linear behavior is important for the **superfluid** behavior of the system. According to Landau, $\min_q (E_q(N) - E_0(N))/|q|$ is, in fact, the **critical velocity** for frictionless flow.

Generalizations and Extensions

- **[Lewin, Nam, Serfaty, Solovej, 2014]** extended this result to more general types of kinetic energy and interaction operators (with less control on the error terms, however)

- In the translation invariant case, **[Dereziński, Napiórkowski, 2014]** studied the case of weakly N-dependent v, scaling to a δ-function as $N \to \infty$ (or, equivalently, the case of large volume)

- Generalized to potentials of the form $N^{-1+3\beta}v(N^\beta x)$ with $0 \leq \beta \leq 1$ by **[Boccato, Brennecke, Cenatiempo, Schlein, 2017–2019]**

- Degenerate Hartree minimizers, as well as **collective excitations**, where condensation occurs in a (non-linear) excited state of the Hartree functional [Nam, S, 2015]

- Bogoliubov correction to the Hartree dynamics of bosons (**[Lewin, Nam, Schlein, 2013] . . .**)

- In the Hartree regime, an expansion to all orders in $1/N$ is possible **[Boßmann, Petrat, S, 2020]**. (Related work by **[Pizzo 2015]**.)

Ideas in the Proof

The proof consists of **two main steps**:

1. Map $L^2_{\rm sym}(\mathbb{R}^{3N})$ to $\mathcal{F}_\perp^{\leq N} \subset \mathcal{F}_\perp$, the Fock space over the orthogonal complement of ϕ_0, via

$$\Psi = \sum_{n=0}^{N} \psi_n \otimes \phi_0^{\otimes N-n} \,, \quad U\Psi = \{\psi_0, \dots, \psi_N, 0, \dots\}$$

It satisfies, for $f, g \perp \phi_0$,

$$\begin{aligned} U a^\dagger(f) a(g) U^\dagger &= a^\dagger(f) a(g) \\ U a^\dagger(\varphi_0) a(g) U^\dagger &= \sqrt{N - \mathbb{N}_\perp}\, a(g) \\ U a^\dagger(\varphi_0) a(\varphi_0) U^\dagger &= N - \mathbb{N}_\perp \end{aligned}$$

2. Show that $U(H_N - NE^{\rm H})U^\dagger$ is well approximated by the Bogoliubov Hamiltonian $H^{\rm Bog}$, i.e, terms of higher order than quadratic are negligible compared to the main terms, at least at low energy.

Conclusions

- Rigorous bounds on the **excitation spectrum** of an interacting Bose gas, in a suitable limit of weak, long-range interactions.
- **Extensions** to dilute gases with short-range interactions are possible (but are much more complicated).
- With the notable exception of exactly solvable models in one dimension, these are the only models where rigorous results on the excitation spectrum are available.
- Verification of Bogoliubov's prediction that the spectrum consists of elementary excitations, with energy that is linear in the momentum for small momentum. In particular, **Landau's criterion for superfluidity** is verified.
- **For the future:** thermodynamic limit, relation to superfluidity, fermionic systems ...