Arbeitsgemeinschaft mini-lecture: Mean-field limit for bosons & Bogoliubov approximation

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In this lecture we will present the Bogoliubov approximation, which is at the heart of the Bogoliubov theory. The aim is to give the intuitive ideas behind this theory in a clear but non-rigorous manner, before Jinyeop Lee proves rigorously the technical details in the next talk.

To make the heuristics more understandable, we consider a simple physical setting. More precisely, we use a box $\Omega = [0,1]^d$, $d \geq 1$, with periodic boundary conditions, containing N particles subject to the Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \ \text{ acting on } L^2_s(\Omega^N).$$

We consider here symmetric functions, i.e. a bosonic system, though the ideas are exactly the same for fermions. We focus on the mean-field regime, but the ideas we present work for other regimes, including the thermodynamic limit and Gross-Pitaevskii.

The potential is assumed to be

- real-valued, i.e. $V : \mathbb{R}^d \to \mathbb{R}$,
- periodic, with period 1: $V(x+n) = V(x)$ for $\forall n \in \mathbb{Z}^d$, $x \in \Omega$,
- bounded: $\|V\|_\infty < \infty$,
- semi-positive definite: $\hat{V}(k) \geq 0$, $\forall k \in 2\pi\mathbb{Z}^d$, where

$$\hat{V}(k) := \int_\Omega V(x) e^{-ik\cdot x} dx.$$

The Bogoliubov theory can be used to estimate the ground state energy of a particle system in the case of interactions, defined by

$$E_N := \inf_{\psi \in L^2_s(\Omega^N):\ \|\psi\|_{L^2}=1} \left\langle \psi \middle| H_N \psi \right\rangle.$$

The first part of the lecture is about finding the ground state energy of the system in the noninteracting case $V \equiv 0$. It can be shown that $E_N = 0$, and a minimizer is $\psi_N^0 = \varphi_0 \otimes \cdots \otimes \varphi_0$ with $\varphi_0 \equiv 1$ on Ω.

The second part of the lecture consists in obtaining an estimate for the ground state energy in the interacting case $V \not\equiv 0$. A first estimate of E_N can be obtained in a straightforward manner by obtaining lower and upper bounds, yielding

$$\left| \frac{N}{2} \hat{V}(0) - E_N \right| \leq C.$$

The upper bound is obtained by using ψ_N^0 as a trial state, and the lower bound comes from a lower bound on V that one can obtain using our assumptions. The lower bound on V can also be used to show that, for wave functions with an energy that remain a constant away from E_N for all N, there is condensation in the state φ_0 as $N \to \infty$. The above estimate of E_N is of order $\mathcal{O}(N)$. To obtain a more precise value, we use the formalism of second quantization using the creation and annihilation operators a_p^*, a_p associated to the Fourier mode of frequency p. We recall that $a_p^* a_p$ is the operator that counts the number of particles in the Fourier mode of frequency p.

The essential idea from Bogoliubov is that, since one expects condensation in the state φ_0 (which is the Fourier mode of frequency 0), one should have $a_0^* a_0 \psi_N \approx N \psi_N$. The operators a_0^*, a_0 don't commute, however $[a_0, a_0^*] = 1 \ll N$. Hence, compared to N, the non-commutability is negligible. Bogoliubov suggests to treat these operators as scalars, with $a_0 = a_0^* = \sqrt{N_0}$ and N_0 the number of particles in the state φ_0. After writing the second quantization of the Hamiltonian H_N and replacing every occurence of the operators a_0, a_0^* with $\sqrt{N_0}$, one obtains an expression with products of two, three, and four creation and annihilation operators. It can be shown that the terms involving products of three and four such operators are of order $N^{-1/2}$, thus become negligible as $N \to \infty$.

In order to treat the products of two creation and annihilation operators, we introduce modified creation and annihilation operators b_p^*, b_p, such that the quadratic part of the second quantized version of H_N becomes diagonal – in the sense that it only involves products of the form $b_p^* b_p$. By writing the Hamiltonian using these new operators, a constant of order $\mathcal{O}(1)$ appears. Finally, the improved estimate of E_N is the addition of the $\mathcal{O}(N)$ and $\mathcal{O}(1)$ estimates of E_N, and other terms in the Hamiltonian vanish as $N \to \infty$.

The theory and computations are the same for bosonic and fermionic systems, up to the definition of the modified operators: these operators b_p^*, b_p have either to satisfy the CCR (in the case of bosons) or CAR (in the case of fermions).

References

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