Bogoliubov theory at positive temperatures

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Introduction

A proof of the existence of a Bose-Einstein Condensation phase transition for a continuous, translation-invariant system in the thermodynamic limit at positive temperature remains an open problem.

Only approximations to the full bosonic many-body problem are considered and analyzed in that context. Here, we reformulate the Bogoliubov approximation for a weakly-interacting translational-invariant Bose gas as a variational model, and show physically relevant properties of this model.

Free energy:

$$\inf_{\omega} \langle H - TS - \mu \mathcal{N} \rangle_{\omega}$$

$$H = \sum_{p} p^2 a_p^\dagger a_p + \frac{1}{2L^3} \sum_{p,q,k} \widehat{V}(k) a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p .$$

Our approximation: restrict ω to *Bogoliubov trial states*: quasi-free states with added condensate.

"added condensate": $a_0 \mapsto a_0 + \sqrt{L^3 \rho_0}$ $\quad$ ($\rho_0 > 0 \equiv$ BEC)

"quasi-free states": we can use Wick's rule to split $\langle a^\dagger_{p+k} a^\dagger_{q-k} a_q a_p \rangle$ and to determine the expectation values it is enough to know two real (we assume translation invariance) functions:

$$\gamma(p) := \langle a^\dagger_p a_p \rangle \geq 0 \text{ and } \alpha(p) := \langle a_p a_{-p} \rangle.$$

Physical interpretation:

- $\gamma(p)$ describes the momentum distribution among the particles in the system
- $\rho_0 > 0$ can be seen as the macroscopic occupation of the zero momentum state (BEC fraction)
- $\alpha(p)$ describes pairing in the system ($\alpha \neq 0 \Rightarrow$ presence of macroscopic coherence related to superfluidity)

- Grand-canonical free energy functional

$$\mathcal{F}(\gamma,\alpha,\rho_0) = (2\pi)^{-3}\int_{\mathbb{R}^3} p^2\gamma(p)dp - \mu\rho - TS(\gamma,\alpha) + \frac{\hat{V}(0)}{2}\rho^2$$
$$+ \frac{1}{2}(2\pi)^{-6}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \hat{V}(p-q)\left(\alpha(p)\alpha(q)+\gamma(p)\gamma(q)\right)dpdq$$
$$+ \rho_0(2\pi)^{-3}\int_{\mathbb{R}^3} \hat{V}(p)\left(\gamma(p)+\alpha(p)\right)dp.$$

- Domain $\mathcal{D} = \{(\gamma,\alpha,\rho_0)|\gamma \in L^1((1+p^2)dp), \gamma \geq 0, \alpha^{\mathbf{2}} \leq \gamma(\mathbf{1}+\gamma), \rho_0 \geq 0\}$.
- ρ denotes the density $\rho = \rho_0 + (2\pi)^{-3}\int_{\mathbb{R}^3}\gamma(p)dp =: \rho_0 + \rho_\gamma$.
- The entropy functional $S(\gamma,\alpha)$

$$S(\gamma,\alpha) = (2\pi)^{-3}\int_{\mathbb{R}^3}\left[\left(\beta(p)+\frac{1}{2}\right)\ln\left(\beta(p)+\frac{1}{2}\right)\right.$$
$$\left. - \left(\beta(p)-\frac{1}{2}\right)\ln\left(\beta(p)-\frac{1}{2}\right)\right]dp, \qquad \beta := \sqrt{(\frac{1}{2}+\gamma)^2-\alpha^2}.$$

Why should Bogoliubov trial states be any good?

- Bogoliubov's approach yields a quadratic Hamiltonian. Ground and Gibbs states of such Hamiltonians are quasi-free states;
- quasi-free states have already proven to be good trial states for the ground state energy of Bose gases (Lieb–Solovej '01 - '04, Solovej '06, Erdös–Schlein–Yau '08, Giuliani–Seiringer '09, Yau–Yin '09, Boccato–Brennecke–Cenatiempo–Schlein '17 - '18, Brietzke–Solovej '17), and may therefore also be for the free energy.

- Canonical free energy functional

$$\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) = (2\pi)^{-3}\int_{\mathbb{R}^3} p^2\gamma(p)dp - TS(\gamma,\alpha) + \frac{\hat{V}(0)}{2}\rho^2 + \rho_0(2\pi)^{-3}\int_{\mathbb{R}^3}\hat{V}(p)\left(\gamma(p)+\alpha(p)\right)dp + \frac{1}{2}(2\pi)^{-6}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\hat{V}(p-q)\left(\alpha(p)\alpha(q)+\gamma(p)\gamma(q)\right)dpdq$$

  with $\rho_0 = \rho - \rho_\gamma$.
- The canonical minimization problem:

$$F^{\mathrm{can}}(T,\rho) = \inf\{\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0=\rho-\rho_\gamma)|(\gamma,\alpha,\rho_0=\rho-\rho_\gamma)\in\mathcal{D}\}$$

- strictly speaking: not a canonical formulation. The expectation value of the number of particles is fixed.

Some questions of interest:

- existence of minimizers;
- existence of phase transitions, phase diagram;
- if yes, determination of the critical temperature.

Remarks:

- bosonic counterpart of the BCS functional (Hainzl–Hamza–Seiringer–Solovej '08, Hainzl–Seiringer '12, Frank–Hainzl–Seiringer–Solovej '12,...);
- functional first appeared in a paper by Critchley-Solomon '76 but has never been analyzed!
- first rigorous (starting from many-body) results concerning the free energy by Seiringer '08, Yin '10 in 3D, recently Deuchert–Mayer–Seiringer '18 in 2D;
- recently Deuchert–Seiringer-Yngvason '18 proved BEC for a trapped system at positive T

Existence of minimizers

Theorem

There exists a minimizer for the both the canonical and grand-canonical Bogoliubov free energy functional.

Obstacles:

- no a priori bound on $\gamma(p)$ (for fermions $\gamma(p) \leq 1$)
- a minimizing sequence could convergence to a measure which could have a singular part that represents the condensate
- this scenario already included in the construction of the functional through the parameter ρ_0

Phase diagram

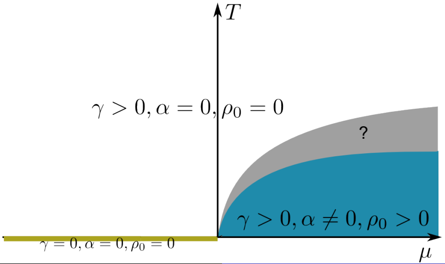
Equivalence of BEC and superfluidity

Let (γ, α, ρ_0) be a minimizing triple for the functional. Then $\rho_0 = 0 \iff \alpha \equiv 0$.

Existence of phase transition

Given $\mu > 0$ ($\rho > 0$) there exist temperatures $0 < T_1 < T_2$ such that a minimizing triple (γ, α, ρ_0) satisfies

1. $\rho_0 = 0$ for $T \geq T_2$;
2. $\rho_0 > 0$ for $0 \leq T \leq T_1$.



Critical temperature in the dilute limit

The dilute limit:

$$\rho^{1/3} a \ll 1$$

where a is the scattering length of the potential.

a describes the **effective range** of the two-body interaction:

$$8\pi a = \int V w$$

where

$$-\Delta w + \frac{1}{2} V w = 0, \qquad w(\infty) = 1$$

Thus

$$a \ll \rho^{-1/3}$$

means range of interaction is much smaller than the mean inter-particle distance.

Expectation for low temperatures $T < D\rho^{2/3}$

dilute gas $\Rightarrow$ weakly interacting $\Rightarrow$ critical temperature close to the critical temperature of the *free Bose gas*

Theorem

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + h(\nu)(\rho^{1/3}a) + o(\rho^{1/3}a)),$$

where $\nu = \widehat{V}(0)/a$ and $h(8\pi) = 1.49$.

This confirms the general prediction that

$$\frac{\Delta T_{\mathrm{c}}}{T_{\mathrm{fc}}} \approx c\rho^{1/3}a$$

with $c > 0$. Here $\Delta T_{\mathrm{c}} = T_{\mathrm{c}} - T_{\mathrm{fc}}$, with T_{c} being the critical temperature in the interacting model and $T_{\mathrm{fc}} = c_0\rho^{2/3}$.
Numerical simulations: $c \sim 1.32$.

Main steps of the proof:

- comparison with the non-interacting case, a priori estimates on the critical density
- in the critical region: introduction of an approximating, simplified functional that can be solved explicitly:

$$\inf_{\substack{(\gamma,\alpha,\rho_0)\\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\text{can}} \approx \inf_{0\le\rho_0\le\rho} \inf_{\substack{(\gamma,\alpha)\\ \rho_\gamma=\rho-\rho_0}} \mathcal{F}^{\text{sim}}$$

Remark:

- a parallel computation in 2D yields the (B)KT transition temperature:

$$T_{\text{c}} = 4\pi\rho\left(\frac{1}{\ln(\xi/4\pi b)} + o(1/\ln^2 b)\right)$$

  with $\xi = 14.4$ and $b = 1/|\ln(\rho a^2)| \ll 1$.
- within this model we interpret this as the transition temperature from a quasicondensate without superfluidity to superfluid quasicondensate
- rigourous upper bounds on T_c in 2D and 3D by Seiringer-Ueltschi '09

Conclusions:

- variational model of interacting Bose gas at positive temperatures;
- can be treated rigorously;
- in the dilute limit leads to physically relevant results (in particular, critical temperature estimates)

Outlook:

- superfluidity (Landau criterion,....);
- waiting for experiments!

Literature: existence and phase diagram $\rightarrow$ ARMA 2018;
dilute limit and critical temperature $\rightarrow$ CMP 2018;
2D critical temperature $\rightarrow$ EPL 2018

Thank you for your attention!