Bogoliubov theory at positive temperatures

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Introduction

General goal: describe properties of a continuous, translation-invariant system of bosons in the thermodynamic limit at positive temperature.

Hamiltonian:

$$H_\Lambda = \sum_{i=1}^{N} -\Delta_i + \sum_{i<j} V(x_i - x_j)$$

acting on $L^2_{\text{sym}}([-L/2, L/2]^d N)$. We assume periodic boundary conditions and consider the limit of both $N, L \to \infty$ with density $\rho := N/L^3$ fixed.

Free energy:

$$\inf_\Gamma (\mathrm{Tr}(H\Gamma) - TS(\Gamma)).$$

In particular, we want to prove **Bose–Einstein Condensation**.

Definition: BEC when the one-body reduced density matrix $\gamma_\Gamma(x, y)$ has an eigenvalue that does not vanish in the thermodynamic limit (macroscopic occupation of a quantum state).

Recall the result mentioned by Nicolas Rougerie:

$$\gamma_\psi \approx |u^{MF}\rangle\langle u^{MF}|.$$

In our setup $u^{MF} \approx L^{-3/2}$. Furthermore

$$\gamma(x, y) = \gamma(x - y) \quad \to \quad \hat{\gamma}(p) \approx \rho_0 \delta_0(p).$$

In terms of creation and annihilation operators:

$$\gamma(x, y) = \langle a_x^* a_y \rangle \rightsquigarrow \hat{\gamma}(p) = \langle a_p^* a_p \rangle.$$

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.

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

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

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

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

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

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)

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.

- Grand-canonical free energy functional

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

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

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

- 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

Main steps of the proof

Step 1. It is enough to prove the existence of minimizers for the auxiliary problem

$$F^{\mathsf{aux}}(\lambda, \rho_0) = \inf \left\{ \mathcal{F}^{\mathrm{aux}}(\gamma, \alpha, \rho_0) \;\middle|\; \int \gamma(p)dp = \lambda, (\gamma, \alpha) \in \mathcal{D}' \right\}$$

where

$$\mathcal{F}^{\mathsf{aux}} = \mathcal{F} + \mu\rho - \frac{\widehat{V}(0)}{2}\rho^2$$

and

$$\mathcal{D}' = \{(\gamma, \alpha) \mid \gamma \in L^1((1+p^2)dp),\ \gamma(p) \geq 0,\ \alpha(p)^2 \leq \gamma(p)(\gamma(p)+1)\}.$$

Advantage: auxiliary functional is jointly convex in (γ, α).

Step 2. Dual problem of the auxiliary problem (which is a restricted minimization) on a smaller domain

$$\mathcal{M}_\kappa = \{(\gamma, \alpha) \in \mathcal{D}' | \gamma(p) \leq \frac{\kappa}{p^2}\}.$$

Artificial a priori bound is used to prove the existence of minimizers for this restricted problem.

Step 3. Construct a minimizing sequence of the unrestricted problem out of the minimizers γ_κ of the restricted problem in the limit $\kappa \to \infty$.

- we show that if there is condensation then only for $p = 0$ (we prove uniform bounds on γ_κ for $|p| > p_\kappa$ with $p_\kappa \to 0$
- we show that mass accumulation at $p = 0$ is impossible for a minimizer since this would increase the energy compared to a solution where the mass would be added to ρ_0 right from the beginning.

Phase diagram

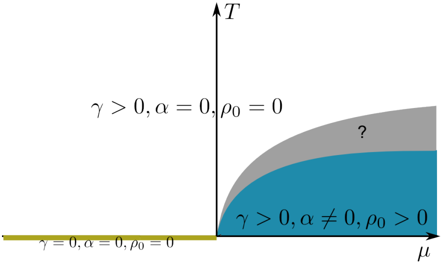
Equivalence of BEC and superfluidity

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

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

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

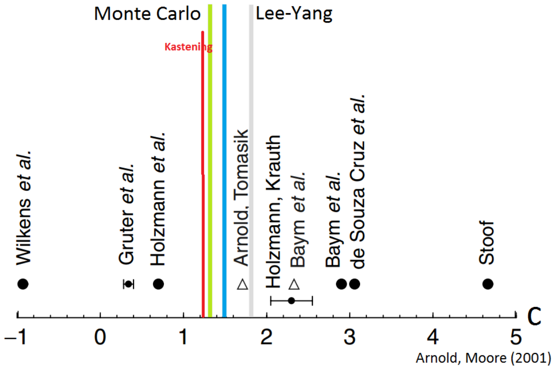
where $\nu = \widehat{V}(0)/a$ and $h(8\pi) = 1.49$.

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: $c \sim 1.32$.

Rigourous upper bounds on T_c in 3D by Seiringer-Ueltschi '09



Critical temperature in two dimensions

It follows from the **Mermin-Wagner theorem** that in two spatial dimensions there is **no BEC** in the sense of exponential decay of correlations functions.

However, as pointed out by Popov (1983), Kagan (1987),...., Castin–Mora (2001) in 2D we have a **quasicondensate**.

Concept of quasicondensate:

- system can be divided into blocks of size $L < R$;
- in each block one can introduce the wave-function of the condensate with a well-defined phase;
- whole system is described in terms of an ensemble of wave-functions of the blocks;
- condensate wave-functions within the ensemble corresponding to blocks separated by a distance greater than R have uncorrelated phases.

Phase transitions in 2D Bose gas:

- from thermal (normal gas), to quasicondensate without superfluidity;
- from quasicondensate without superfluidity to superfluid quasicondensate **(BKT transition)**

Recall, in our model,

$$\text{BEC} \equiv \text{superluidity}$$

We see only the BKT transition! We compute

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

with $\xi = 14.4$.

Remarks:

- Fisher–Hohenberg 1988 computed/estimated the leading order term for the first time (ξ not determined);
- first analytical computation of the constant ξ (to our knowledge);
- numerical prediction of $\xi = 380$ Prokof'ev–Ruebenacker–Svistunov 2001,
- like Schick 1971 (ground state) we need **diluteness parameter**

$$b = 1/|\ln(\rho a^2)| \ll 1$$

unlike Popov, Fisher-Hohenberg,... who need $\ln(1/b) \gg 1$.

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,....);
- better understanding of the 2D model (ground state energy expansion);
- 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!