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:

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

Free energy:

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

Thermodynamic limit:

$$\rho = \frac{N}{L^3} = const., \quad N, L \to \infty.$$

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

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

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

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

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

- Canonical free energy functional

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

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

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

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

Some questions of interest:

- existence of minimizers;
- free energy asymptotics;
- existence of Bose–Einstein condensation (phase diagram);
- if yes, determination of the critical temperature.

Rigorous results from Many-Body QM:

- energy: Lieb–Yngvason, Erdös–Schlein–Yau, Yau–Yin, Seiringer–Giuliani,..., Boccato-Brennecke-Cenatiempo-Schlein, Solovej–Fournais;
- free energy: Seiringer, Yin, recently Deuchert–Mayer–Seiringer, Mayer–Seiringer;
- BEC: results on hard-core bosons Kennedy-Shastry-Lieb, Aizenman-Lieb-Seiringer-Solovej-Yngvason, recently Deuchert–Seiringer proved BEC at positive T, but thermodynamic limit still open!
- critical temperature: Seiringer–Ueltshi upper bound.

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

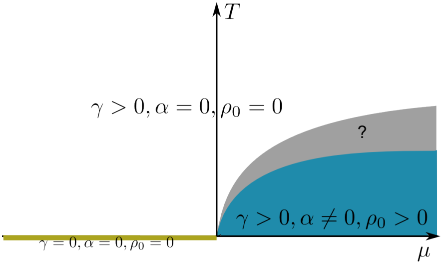
Equivalence of BEC and superfluidity

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

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 $0 \leq T \leq T_1$.



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.

Simplified functional

Main idea:

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

The explicit minimization in γ and α has to be done for

$$\int_{\mathbb{R}^3} p^2\gamma(p)dp - TS(\gamma,\alpha) + \rho_0 \int_{\mathbb{R}^3} \widehat{Vw}(p)\left(\gamma(p)+\alpha(p)\right)dp$$

which results in integrals that depend on ρ and ρ_0.

Convolution terms contribute in a linearized way to give $\widehat{Vw}$.

Free energy asymptotics

In the dilute limit $\rho^{1/3}a \ll 1$ and when $T \ll \rho a$ (low temperature expansion)

$$F^{\mathrm{can}}(\rho, T) = 4\pi\rho^2 a \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a_{\mathrm{B}}^3} + o(\sqrt{\rho a^3}(1 + T/(\rho a)))\right)$$

Remarks:

- here a_{B} depends on V and $a_{\mathrm{B}} \approx a$ when $\int V \approx 8\pi a$;
- this is an extension of the Erdös–Schlein–Yau result mentioned earlier;
- the Lee–Huang–Yang formula has recently been finally proved after 60 years by Fournais–Solovej (lower bound, earlier upper bound by Yau-Yin)

Critical temperature

Ideal gas:

$$T_{\mathrm{fc}} = c_0 \rho^{\frac{2}{3}}.$$

Question: how does the interaction change the critical temperature?

- 1953 Feynman predicted for liquid helium $\Delta T_c < 0$;
- 1958 Lee-Yang computed for hard-sphere Bose gas in the dilute limit

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + 1.79(\rho^{1/3}a) + o(\rho^{1/3}a))$$

- rigourous result: Seiringer–Ueltschi:

$$T_{\mathrm{c}} \leq T_{\mathrm{fc}}(1 + 5.09\sqrt{\rho^{1/3}a})$$

We show:

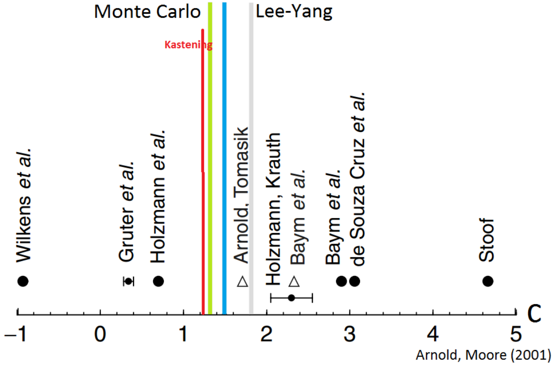
$$\boxed{T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + 1.49(\rho^{1/3}a) + o(\rho^{1/3}a))}$$

General prediction that

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

with $c > 0$.

Numerical (QMC) simulations: $c \sim 1.32$.

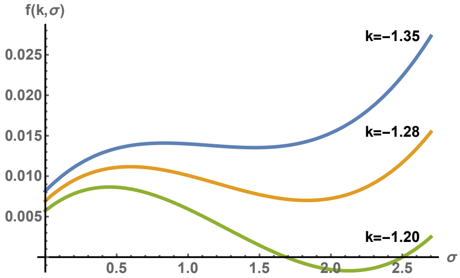


Idea behind the proof

$$\rho_0 = \frac{\sigma}{8\pi} T^2 a \qquad\qquad \rho = \rho_{\text{fc}} + \frac{k}{8\pi} T^2 a$$

and **expanding** the integrals for $\sqrt{T}a \approx \rho^{1/3} a \ll 1$ reduces the problem to minimizing an explicit f in σ:

$$\inf_{\substack{(\gamma,\alpha,\rho_0)\\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\text{can}} \approx \inf_{0\leq\rho_0\leq\rho} \left[\inf_{\substack{(\gamma,\alpha)\\ \rho_\gamma=\rho-\rho_0}} \mathcal{F}^{\text{sim}} \right] \approx f_0(T,\rho) + T^4 a^3 \inf_{\sigma\geq 0} f(k,\sigma)$$



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 $\xi = 14.4$.

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,....);
- understanding of the 1D model;
- waiting for experiments!

Open: postdoc position in analysis of Bose gases, in collaboration with Phan Thanh Nam (LMU Munich), contact me directly!

Thank you for your attention!