The Gibbs state of the mean-field Bose gas and a new correlation inequality

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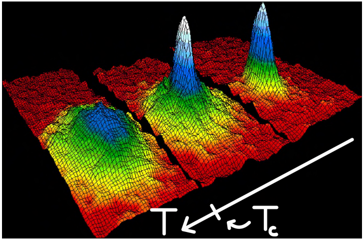
A gas of quantum mechanical particles

Background: Bose–Einstein condensation (BEC)



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Wolfgang Ketterle, Nobel Prize in Physics in 2001.

Interacting Bose gases display wealth of interesting phenomena related to the BEC phase transition, that are notoriously difficult to study mathematically because:

- Curse of dimensionality ⇒ Analysis extremely challenging (in experiments $N \approx 10^3 - 10^6$),
- Small denominator problem ⇒ Perturbation theory fails in interacting many-body quantum systems.

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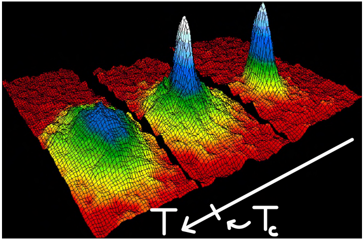

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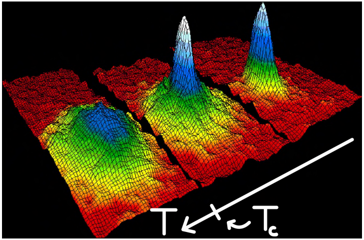

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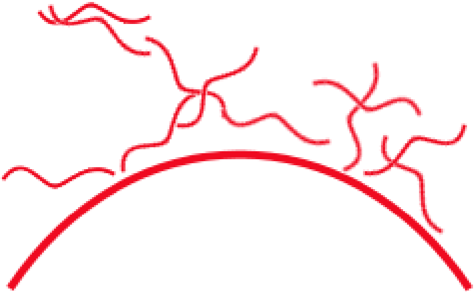
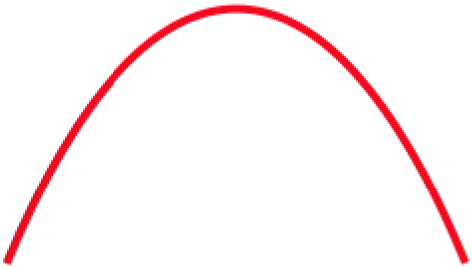
Above the critical point

Below the critical point



At zero temperature



Starting point: the microscopic model

We are interested in a system of bosons captured in the unit torus with fluctuating particle number. The Hilbert space of the system is therefore the bosonic Fock space

$$\mathscr{F}(L^2([0,1]^3) = \bigoplus_{n=0}^{\infty} L^2_{\text{sym}}([0,1]^{3n}).$$

Here $L^2_{\text{sym}}([0,1]^{3n})$ denotes the set of all L^2-functions that satisfy

$$\Psi(x_1, ..., x_i, ..., x_j, ..., x_n) = \Psi(x_1, ..., x_j, ..., x_i, ..., x_n) \quad \forall\ i < j.$$

The Hamiltonian of the system reads

$$\mathcal{H}_N = 0 \bigoplus_{n=1}^{\infty} \left[\sum_{i=1}^{n} -\Delta_j + \frac{1}{N} \sum_{1 \leq i < j \leq n} v(x_i - x_j) \right].$$

Here $v \in L^1$ is nonnegative and N denotes the expected particle number.

Creation and annihilation operators

By a_p^* and a_p we denote the creation and annihilation operators on $\mathscr{F}$ that create and annihilate a particle in the function $\varphi_p(x) = e^{\mathrm{i}p\cdot x}$ with $p \in 2\pi\mathbb{Z}^3$, respectively. That is,

$$(a_p^* \Psi_n)(x_1, ..., x_n, x_{n+1}) = \mathrm{Sym}[\varphi_p(x_{n+1})\Psi_N(x_1, ..., x_n)].$$

They satisfy the canonical commutation relations (CCR)

$$[a_p, a_q^*] = \delta_{p,q}, \qquad [a_p, a_q] = 0 = [a_p^*, a_q^*].$$

The Hamiltonian can be written as

$$\mathcal{H}_N = \sum_{p \in 2\pi\mathbb{Z}^3} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,u,v \in 2\pi\mathbb{Z}^3} \hat{v}(p) a_{u+p}^* a_{v-p}^* a_u a_v$$

with the Fourier coefficients $\hat{v} \geq 0$ of v.

Free energy and Gibbs state

Equilibrium properties of the system are encoded in the free energy

$$F(\beta, N) = -\frac{1}{\beta} \ln \left(\operatorname{Tr} \exp(-\beta(\mathcal{H}_N - \mu \mathcal{N})) \right) + \mu N$$

at inverse temperature $\beta > 0$ and the Gibbs state

$$G_{\beta,N} = \frac{\exp(-\beta(\mathcal{H}_N - \mu \mathcal{N}))}{\operatorname{Tr} \exp(-\beta(\mathcal{H}_N - \mu \mathcal{N}))}.$$

The chemical potential μ is chosen s.t.

$$\operatorname{Tr}[\mathcal{N} G_{\beta,N}] = N$$

holds.

Parameter regime: $N \to \infty$, $\beta = \kappa \beta_c$ with $\beta_c = \frac{1}{4\pi} \left(\frac{N}{\zeta(3/2)} \right)^{-2/3}$ and $\kappa \in (0, \infty)$.

Bose–Einstein condensation in the ideal gas

Let $v = 0$ and denote by

$$N_0(\beta, N) = \mathrm{Tr}[a_0^* a_0 G_{\beta,N}]$$

the expected number of particles in the constant function.

It has the aymptotic behavior

$$N_0(\beta, N) = \frac{1}{\exp(-\beta\mu_0) - 1} \simeq N \left[1 - \left(\frac{\beta_c}{\beta}\right)^{3/2}\right]_+ \quad \text{with}$$

$$\beta_c = \beta_c(N) = \frac{1}{4\pi}\left(\frac{N}{\zeta(3/2)}\right)^{-2/3}$$

in the limit $N \to \infty$. This behavior persits in the interacting model (reference on next page)!

Literature

Low lying excitation spectrum

- Seiringer, Commun. Math. Phys. (2011)
- Lewin, Nam, Serfaty, Solovej, Commun. Pure Appl. Math. (2015)
- Nam, Seiringer, Arch. Rational Mech. Anal. (2015)

BEC and dependence of critical temperature for BEC on interaction

- D., Seiringer, Yngvason, Commun. Math. Phys. (2019)
- D., Seiringer, Arch. Rational Mech. Anal. (2020)
- D., Seiringer, J. Funct. Anal. (2021)

Derivation of nonlinear Gibbs measures

- Lewin, Nam, Rougerie, Invent. Math. (2021)
- Fröhlich, Knowles, Schlein, Sohinger, JAMS (2022)

Theorem 1 (Convergence of Gibbs state)

The Gibbs state $G_{\beta,N}$ is close (in trace norm) to the state

$$\Gamma = \int_{\mathbb{C}} |z\rangle\langle z| \otimes G^{\mathrm{Bog}}(z) g^{\mathrm{BEC}}(z)\,\mathrm{d}z,$$

on $\mathscr{F} \simeq \mathscr{F}_0 \otimes \mathscr{F}_+$ with the coherent state $|z\rangle = \exp(za_0^* + \bar{z}a_0)|\Omega\rangle$.

Here $G^{\mathrm{Bog}}(z)$ is the Gibbs state of the Bogoliubov Hamiltonian

$$\mathcal{H}^{\mathrm{Bog}}(z) = \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} p^2 a_p^* a_p + \frac{N_0(\beta,N)}{2N} \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} \hat{v}(p) \left(2a_p^* a_p + (z/|z|)^2 a_p^* a_{-p}^* + (\bar{z}/|z|)^2 a_p a_{-p}\right)$$

and the condensate is described by

$$g^{\mathrm{BEC}}(z) \propto \exp(-\beta(\hat{v}(0)/(2N)|z|^4 - \mu^{\mathrm{BEC}}|z|^2)).$$

Theorem 2 (Distribution of condensate particle number)

The distribution of the number of particles in the condensate

$$p^{\text{Gibbs}}(n) = \operatorname{Tr}[|n\rangle\langle n| \otimes \mathbb{1}_+ G_{\beta,N}],$$

where

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(a_0^*\right)^n |\text{vac}\rangle,$$

satisfies

$$\lim_{N\to\infty} \sum_{n=0}^{\infty} \left| p^{\text{Gibbs}}(n) - g\left(\frac{n - N_0(\beta, N)}{\sqrt{\frac{N}{\beta \hat{v}(0)}}} \right) \right| = 0$$

with the normal distribution $g(x) = (2\pi)^{-3/2} \exp(-x^2/2)$.

Theorem 3 (Two-particle density matrix)

Matrix elements of two-particle density matrix of Gibbs state converge to that of Γ. Selected implications: The variance of the number of particles in the condensate satisfies

$$\mathrm{Tr}[a_0^* a_0 a_0^* a_0 G_{\beta,N}] - (\mathrm{Tr}[a_0^* a_0 G_{\beta,N}])^2 = \frac{N}{\beta \hat{v}(0)}(1 + o(1)).$$

Moreover,

$$\begin{aligned} \mathrm{Tr}[a_0^* a_0^* a_p a_{-p} G_{\beta,N}] &= N_0(\beta, N)\alpha_{\beta,N}(p)(1 + o(1)), \\ \mathrm{Tr}[a_p^* a_{-p}^* a_p a_{-p} G_{\beta,N}] &= \alpha_{\beta,N}^2(p)(1 + o(1)), \end{aligned}$$

where $N_0(\beta, N)$ is the number of particles in the condensate and $\alpha_{\beta,N}$ is the pairing function of a Bogoliubov Gibbs state.

Theorem 4 (A new abstract correlation inequality)

Let A be self-adoint, let B be symmetric and assume that

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$$

with $0 < a < 1$ and $b \geq 0$. Assume additionally that $\exp(-(1-a)A)$ is trace-class and that the state

$$\Gamma_t = \frac{\exp(A+tB)}{\mathrm{Tr}[\exp(A+tB)]} \quad \text{satisfies} \quad \sup_{t\in[-1,1]} |\,\mathrm{Tr}[B\Gamma_t]| \leq \eta$$

for some constant $\eta > 0$. Then we have

$$\mathrm{Tr}[B^2\Gamma_0] \leq \eta\exp(\eta) + \frac{1}{4}\,\mathrm{Tr}([[B,A],B])\Gamma_0).$$

This greatly simplifies and generalizes a correlation inequality in Lewin, Nam, Rougerie, Invent. Math. (2021).

Theorem 5 (An infnite-dimensional version of Stahl's theorem)

Let A be self-adoint, let B be symmetric and assume that

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$$

holds $0 < a < 1$ and $b \geq 1$. Assume additionally that $\exp(-(1-a)A)$ is trace-class and define ($t \in [-1, 1]$)

$$Z(t) = \mathrm{Tr}[\exp(-(A + tB))].$$

Then there exists a nonnegative Borel measure μ such that

$$Z(t) = \int_{-\infty}^{\infty} e^{-ts}\, \mathrm{d}\mu(s)$$

holds.

References (Stahl's theorem f.k.a. BMV conjecture):

- Bessis, Moussa, Villani, J. Math. Phys. (1975)
- Stahl, Acta Math. (2013)

Proof of Correlation inequality with Stahl's Theorem

By assumption we have ($t \in [-1, 1]$)

$$|\partial_t \ln(Z(t))| = |\operatorname{Tr}[B\Gamma_t]| \leq \eta \quad \Rightarrow \quad Z(t) \leq e^{\eta} Z(0).$$

An application of Stahl's theorem shows $Z^{(4)}(t) \geq 0$, and hence the Duhamel-two-point function

$$Z''(t) = \int_0^1 \operatorname{Tr}\left[Be^{-(A+tB)s} Be^{-(A+tB)(1-s)}\right] \mathrm{d}s$$

is convex! But this implies

$$Z''(0) \leq \frac{1}{2} \int_{-1}^{1} Z''(s)\, \mathrm{d}s \leq \sup_{t \in [-1,1]} Z'(t) \leq \eta e^{\eta} Z(0).$$

Finally, an application of the Falk–Bruch inequality shows

$$\operatorname{Tr}[B^2 \Gamma_0] \leq \frac{Z'(0)}{Z(0)} + \operatorname{Tr}([[B, A], B]\Gamma_0).$$

Summary

- Approximation of Gibbs state in trace norm.
- Computation of 2-pdm and condensate distribution.
- New abstract correlation inequality.
- Infinite-dimensional version of Stahl's theorem.