Gross-Pitaevskii limit of a homogeneous Bose gas at positive temperature

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The homogeneous Bose gas in experiments

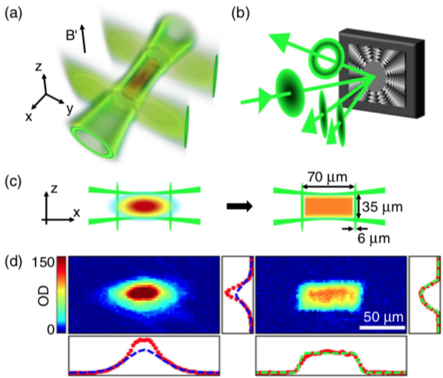

Figure: A. L. Gaunt, T. F. Schmidutz, I. Gotlibovych, R. P. Smith, Z. Hadzibabic, Phys. Rev. Lett. **110**, 200406 (2013)

Also possible: 2d Bose gas, 2d and 3d Fermi gases.

The ideal Bose gas

Consider the ideal Bose gas on $[0, L]^3$ with periodic boundary conditions. The **expected number of particles** in the grand canonical ensemble is given by

$$N = \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{\exp\left(\left(p^2 - \mu\right)/T\right) - 1}.$$

Here $\mu(T, N, L)$ and T denote the chemical potential and the temperature.

The expected number of particles in the Bose-Einstein condensate (BEC) $N_0(T, N, L) = [e^{-\mu/T} - 1]^{-1}$ is, as $N \to \infty$, to leading order given by

$$\frac{N_0(T, N, L)}{N} \simeq \left[1 - \left(\frac{T}{T_{\mathrm{c}}}\right)^{3/2}\right]_+ \qquad \text{with} \qquad T_{\mathrm{c}} = 4\pi \left(\frac{N/L^3}{\zeta(3/2)}\right)^{2/3}.$$

The Hamiltonian of the interacting model

Hamiltonian with Gross-Pitaevskii scaling:

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \leq i < j \leq N} L^{-2} N^2 v\left(N|x_i - x_j|/L\right).$$

Here Δ is the Laplacian on $[0, L]^3$ with periodic boundary conditions and $v \geq 0$ such that scattering length is finite.

The **scattering length** a_N of $L^{-2} N^2 v\left(N|x|/L\right)$ behaves as

$$a_N \sim L N^{-1} \quad \Rightarrow \quad a_N \ll \varrho^{-1/3}.$$

Free energy and Gibbs variational principle

The **free energy** of the gas is given by

$$F(T,N,L) = -T \ln\left(\operatorname{Tr}\left[e^{-H_N/T}\right]\right),$$

where the trace is taken over functions that are symmetric under an exchange of the coordinates.

Gibbs variation principle: Let

$$\mathcal{S}_N = \left\{\Gamma \in \mathcal{L}\left(L^2_{\mathrm{sym}}\left(\mathbb{R}^{3N}\right)\right) \,\middle|\, 0 \leq \Gamma \leq 1 \text{ and } \operatorname{Tr}\Gamma = 1\right\},$$

then

$$F(T,N,L) = \inf_{\Gamma \in \mathcal{S}_N} \underbrace{\left\{\operatorname{Tr}\left[H_N \Gamma\right] - TS(\Gamma)\right\}}_{=\mathcal{F}(\Gamma)} \quad \text{with} \quad S(\Gamma) = -\operatorname{Tr}\left[\Gamma \ln(\Gamma)\right].$$

1-pdm and Bose-Einstein condensation

The **one-particle reduced density matrix (1-pdm)** of a state $\Gamma \in \mathcal{S}_N$ can be defined via its integral kernel by

$$\gamma(x, y) = \mathrm{Tr}\left[a_y^* a_x \Gamma\right].$$

Here a_x^* and a_x denote the usual creation and annihilation operators.
Equivalently, this kernel can be defined by

$$\gamma(x, y) = N \int_{\mathbb{R}^{3(N-1)}} \Gamma(x, q_1, \ldots, q_{N-1}; y, q_1, \ldots, q_{N-1}) \mathrm{d}(q_1, \ldots, q_{N-1}).$$

A sequence of states $\Gamma_N \in \mathcal{S}_N$ with 1-pdms γ_N is said to show **Bose-Einstein condensation (BEC)** if

$$\liminf_{N \to \infty} \sup_{\|\phi\|=1} \frac{\langle \phi, \gamma_N \phi \rangle}{N} > 0.$$

Mathematical literature on dilute Bose gases, $T = 0$

- **Ground state asymptotics of dilute Bose gas in thermodynamic limit**: Dyson '57 (Upper bound hard spheres), Lieb, Yngvason '98 (Lower bound), Lieb, Seiringer, Yngvason '00 (General upper bound)
- **LHY formula**: Yau, Yin '09 (Upper bound), Fournais, Solovej '19 (Lower bound)
- **Ground state asymptotics in GP limit**: Lieb, Seiringer, Yngvason '00, Lieb, Seiringer '02, Boccato, Brennecke, Cenatiempo, Schlein '17, '18
- **GP limit of rotating Bose gas**: Lieb, Seiringer '06, Nam, Rougerie, Seiringer '16
- **Bogoliubov theory in GP scaling**: Boccato, Brennecke, Cenatiempo, Schlein '18
- **Dynamics of BEC in GP limit**: Erdös, Schlein, Yau '09 and '10, Pickl '15, Benedikter, de Oliveira, Schlein '15

Mathematical literature on dilute Bose gases, $T > 0$

Results in thermodynamic limit:

- Free energy asymptotics of dilute Bose gas in thermodynamic limit: Seiringer '08 (Lower bound)
- Free energy asymptotics of dilute Bose gas in thermodynamic limit: Yin '10 (Upper bound)
- Free energy of quasi-free states in $d = 2, 3$ and critical temperatures: Napiórkowski, Reuvers, Solovej '18, +Fournais '19

Results in GP limit:

- Free energy asymptotics and prove of BEC for trapped gas in GP limit: Deuchert, Seiringer, Yngvason '18

Theorem: Part 1 (Asymptotics of free energy)

Assumptions:

- v a nonnegative, radial and measurable function which is integrable outside some finite ball ($\Leftrightarrow a_N < \infty$)
- Limit: $N \to \infty$, $T \lesssim T_{\mathrm{c}}$ and $a_N \sim LN^{-1}$

Notation:

- $F_0(T, N, L) \sim L^3 T^{5/2} \sim L^{-2} N^{5/3}$ the free energy of the ideal gas
- $\varrho_0(T, N, L) = N_0(T, N, L)/L^3$ expected density of particles in condensate of ideal Bose gas

We have

$$F(T, N, L) = F_0(T, N, L) + 4\pi a_N L^3 \left(2\varrho^2 - \varrho_0 (T, N, L)^2\right)(1 + o(1)).$$

Note that $4\pi a_N L^3 \varrho^2 \sim L^{-2} N$.

Theorem: Part 2 (Asymptotics of 1-pdm)

Notation:

- State Γ_N with 1-pdm γ_N and free energy $\mathcal{F}(\Gamma_N)$
- $\gamma_{N,0}$ denotes 1-pdm of the non-interacting canonical Gibbs state

For any sequence of approximate minimizers Γ_N of the free energy in the sense

$$\mathcal{F}_N(\Gamma_N) = F_0(T,N,L) + 4\pi a_N L^3 \left(2\varrho^2 - \varrho_0(T,N,L)^2\right)(1+o(1))$$

we have

$$\|\gamma_N - \gamma_{N,0}\|_1 = o(N).$$

Remarks

- **Result for 1-pdm implies BEC** in the form

$$\lim_{N\to\infty} \sup_{\|\phi\|=1} \frac{\langle \phi, \gamma_N \phi \rangle}{N} = \left[1 - \left(\frac{T}{T_{\mathrm{c}}}\right)^{3/2}\right]_+$$

  with critical temperature T_{c} of the ideal gas.

- **Quantities related to the ideal gas**, that is, $N_0(T, N, L)$, $\gamma_{N,0}$ and $F_0(T, N, L)$, can be replaced by their **grand canonical versions**.

- **Uniformity in temperature** as long as $T \leq CT_{\mathrm{c}}$ for some $C > 0$.

- Treatment of **Dirichlet boundary conditions** possible.

Ingredients of the proof

- **Upper bound:** Much simpler proof than in thermodynamic limit (Yin '10) possible because the system in the GP scaling is much more dilute (5 vs. 55 pages).
- **Lower bound:** Adaption of the proof of the lower bound in the thermodynamic limit (Seiringer '08) with an error of the same size.
- **Asymptotics of 1-pdm and BEC:** C-number substitution with general state instead of interacting Gibbs state, novel bound for bosonic relative entropy, Griffith argument to detect condensate.

And now some more details concerning the proof...

Proof of upper bound: the trial state

Let

$$\Gamma^{\mathrm{G}} = \frac{e^{-H_N^0/T}}{\mathrm{Tr}\left[e^{-H_N^0/T}\right]} = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

be the **canonical Gibbs state of the ideal gas**. Denote by $f(|x|)$ the solution to the **zero energy scattering equation**

$$-\Delta f(|x|) + \tfrac{1}{2} v_N(|x|) f(|x|) = 0 \quad \text{with} \quad \lim_{|x|\to\infty} f(|x|) = 1$$

and define $f_b(r) = f(r)/f(b)$ if $r < b$ and $f_b(r) = 1$ otherwise. Let $F(x_1, ..., x_N) = \prod_{1 \leq i < j \leq N} f_b(|x_i - x_j|)$. The **trial state** is given by

$$\widetilde{\Gamma}^{\mathrm{G}} = \sum_{\alpha=1}^{\infty} \lambda_\alpha \frac{|F\Psi_\alpha\rangle\langle F\Psi_\alpha|}{\langle F\Psi_\alpha, F\Psi_\alpha\rangle}.$$

Proof of lower bound: coherent states

Pick $p_{\rm c} > 0$ and let $M = \#\{p \in \frac{2\pi}{L}\mathbb{Z}^3 | |p| < p_{\rm c}\}$. For a vector $z \in \mathbb{C}^M$ define the **coherent state**

$$|z\rangle = \exp\left(\sum_{|p|<p_{\rm c}} z_p a_p^* - \overline{z_p} a_p\right)|\mathrm{vac}\rangle.$$

We have $a_p|z\rangle = z_p|z\rangle$ if $|p| < p_{\rm c}$. For a second quantized operator, e.g. $\mathbb{N} = \sum_p a_p^* a_p$, the **lower and upper symbols** are defined by

$$\mathbb{N}_{\rm s}(z) := \langle z, \mathbb{N} z\rangle = \sum_{|p|<p_{\rm c}} |z_p|^2 + \sum_{|p|\geq p_{\rm c}} a_p^* a_p \quad \text{and}$$

$$\mathbb{N} = \int_{\mathbb{C}^M} |z\rangle\langle z| \otimes \mathbb{N}^{\rm s}(z)\,\mathrm{d}z, \;\Rightarrow\; \mathbb{N}^{\rm s}(z) = \sum_{|p|<p_{\rm c}} \left(|z_p|^2 - 1\right) + \sum_{|p|\geq p_{\rm c}} a_p^* a_p,$$

respectively. Here $z_p = x_p + iy_p$ and $\mathrm{d}z = \prod_{|p|<p_{\rm c}} \frac{\mathrm{d}x_p\,\mathrm{d}y_p}{\pi}$.

The c-number substitution

Denote by $\mathbb{H}$ the **second quantized Hamiltonian**

$$\mathbb{H} = \sum_p \left(p^2 - \mu\right) a_p^* a_p + \frac{1}{2L^3} \sum_{p,k,\ell} \hat{v}_N(p) a_{k+p}^* a_{\ell-p}^* a_k a_\ell.$$

For the grand-canonical partition function one has the **Berezin-Lieb inequality**

$$\begin{aligned}\int_{\mathbb{C}^M} \mathrm{Tr}_> \exp\left(-\mathbb{H}_{\mathrm{s}}(z)/T\right) \, \mathrm{d}z &\leq \mathrm{Tr} \exp\left(-\mathbb{H}/T\right) \\ &\leq \int_{\mathbb{C}^M} \mathrm{Tr}_> \exp\left(-\mathbb{H}^{\mathrm{s}}(z)/T\right) \, \mathrm{d}z.\end{aligned}$$

(Berezin '72, Lieb '73).

The c-number substitution with a general state: part 1

For a given state Γ on the Fock space define **the state** Γ_z and **the classical probability distribution** ζ_Γ by

$$\Gamma_z = \frac{\langle z, \Gamma z\rangle}{\mathrm{Tr}_> \langle z, \Gamma z\rangle} \quad \text{and} \quad \zeta_\Gamma(z) = \mathrm{Tr}_> \langle z, \Gamma z\rangle,$$

respectively.

Lemma

The entropy of Γ is bounded by

$$S(\Gamma) \leq \int_{\mathbb{C}^M} S(\Gamma_z)\zeta_\Gamma(z)\,\mathrm{d}z - \int_{\mathbb{C}^M} \ln\left(\zeta_\Gamma(z)\right)\zeta_\Gamma(z)\,\mathrm{d}z.$$

c-number substitution with a general state: part 2

For the **free energy** of a state $\Gamma \in \mathcal{S}_N$ the Lemma implies

$$\operatorname{Tr}[H_N \Gamma] - TS(\Gamma) \geq \mu N + \int_{\mathbb{C}^M} \left\{ \operatorname{Tr}[\mathbb{H}^{\mathrm{s}}(z)\Gamma_z] - TS(\Gamma_z) \right\} \zeta_\Gamma(z) \, \mathrm{d}z - TS(\zeta_\Gamma)$$

where

$$S(\zeta_\Gamma) = -\int_{\mathbb{C}^M} \ln(\zeta_\Gamma(z)) \, \zeta_\Gamma(z) \, \mathrm{d}z$$

is **the entropy of the classical distribution** ζ_Γ.

What about the asymptotics of the one-particle density matrix?

Asymptotics of thermal cloud: part 1

Let Γ_N be a sequence of of **approximate minimizers** in the sense that

$$\mathrm{Tr}\left[H_N \Gamma_N\right] - TS(\Gamma_N) = F_0(\beta, N, L) + 4\pi a_N L^3 \left(2\varrho^2 - \varrho_0^2\right)(1 + o(1))$$

we have

$$\int_{\mathbb{C}^M} \mathcal{S}\left(\gamma_z, \widetilde{\gamma}_0\right) \zeta_\Gamma(z) \, \mathrm{d}z \leq o\left(N^{1/3}\right)$$

where

$$\mathcal{S}(a, b) = \mathrm{Tr}\left[\sigma(a) - \sigma(b) - \sigma'(b)(a - b)\right]$$

with $\sigma(x) = x \ln(x) - (1 + x)\ln(1 + x)$ denotes the **bosonic relative entropy**.

Asymptotics of thermal cloud: part 2

Lemma

There exists a constant $C > 0$ such that for any two nonnegative trace-class operators γ, γ_0 we have

$$\mathcal{S}(\gamma, \gamma_0) \geq C \frac{\|\gamma - \gamma_0\|_1^2}{\|1 + \gamma_0\| \operatorname{Tr}[\gamma + \gamma_0]}.$$

With the Lemma and the bound from the previous slide **one concludes**

$$\|\mathbb{1}(-\Delta \geq p_{\mathrm{c}})(\gamma - \gamma_0)\mathbb{1}(-\Delta \geq p_{\mathrm{c}})\|_1 \leq o(N).$$

The condensate

Prove lower bound with H_N **replaced by**

$$H_N^\lambda = H_N + \lambda \sum_{i=1}^{N} |\Phi\rangle\langle\Phi|_i,$$

where $\Phi(x) = L^{-3/2}$. The **lower bound** then reads

$$\operatorname{Tr}\left[H_N^\lambda \Gamma\right] - TS(\Gamma) \geq F_0(T,N,L,\lambda) + 4\pi a_N L^3 \left(2\varrho^2 - \varrho_0(T,N,L)^2\right) - o(N/L^2)$$

and we conclude

$$\langle \Phi, \gamma \Phi\rangle \geq \frac{F_0(T,N,L,\lambda) - F_0(T,N,L,0)}{\lambda} - \frac{L^3 a_N \varrho^2 o(1)}{\lambda}.$$

$$\Rightarrow \left\| \mathbb{1}\left(-\Delta < p_{\mathrm{c}}\right)\left(\gamma - \gamma_0\right)\mathbb{1}\left(-\Delta < p_{\mathrm{c}}\right)\right\|_1 \leq o(N).$$

Thank you for your attention!