

## Gross–Pitaevskii Limit of a Homogeneous Bose Gas at Positive Temperature

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(joint work with Robert Seiringer)

The experimental realization of Bose–Einstein condensation (BEC) in trapped alkali gases in 1995 [3, 1] triggered numerous experimental, theoretical and mathematical investigations of the properties of dilute quantum gases. While early experiments could only prepare such systems in harmonic traps, modern experimental techniques allow also for the engineering of box-like trapping potentials with approximate Dirichlet boundary conditions at the edges [7].

In a recent work we considered together with Jakob Yngvason the trapped Bose gas in the Gross–Pitaevskii (GP) limit at positive temperature [4]. We were able to prove that the difference between the interacting free energy and the one of the ideal gas is to leading order given by the minimum of a GP energy functional. Additionally, we could show that the one-particle density matrix (1-pdm) of every approximate minimizer of the Gibbs free energy functional is to leading order given by the one of the ideal gas, where the condensate wave function has been replaced by the minimizer of the GP energy functional. The proof of these statements is based on the fact that particles inside the thermal cloud live on a much larger length scale than particles inside the condensate, and hence the interaction can be seen to leading order only in the condensate.

The experimentally relevant and mathematically more difficult case of the gas in a box, where the condensate and the non-condensed particles live on the same length scale and all interactions are relevant to leading order, had been left as an open problem. In the remainder of this note we consider this case. More precisely, we consider a system of  $N$  bosonic particles confined in a three-dimensional box of side length  $L$ , whose Hamiltonian reads

$$(1) \quad H_N = \sum_{i=1}^N -\Delta_i + \sum_{1 \leq i < j \leq N} v_N(x_i - x_j).$$

By  $\Delta_i$  we denote the Laplacian with periodic boundary conditions acting on the  $i$ -th particle. With our methods we can also treat Dirichlet boundary conditions but we do not consider this case here. The interaction potential is of the form

$$(2) \quad v_N(x) = (N/L)^2 v(Nx/L),$$

with a nonnegative potential  $v$ . The scattering length  $a_N$  of  $v_N$  scales as  $a_N/L \sim N^{-1}$ , which assures that the interaction energy per particle is of the same order as the spectral gap of the Laplacian in the box. The scattering length is a combined measure for the range and the strength of a potential and it is the only parameter that enters the low energy scattering cross-section in quantum mechanics.

Ground state properties of the dilute Bose gas have been investigated from a mathematical point of view in great detail in the GP limit and in the thermodynamic limit. See [8] for an overview and [2, 6] for two recent developments

concerning the excitation spectrum of the Bose gas in the GP limit and the next-to-leading order correction of the ground state energy in the thermodynamic limit.

In this note we are interested in the Bose gas at positive temperature, and therefore consider the canonical free energy of the system. As the ground state energy, it can be characterized by a variational principle called the Gibbs variational principle. Denote by  $S_N = \{\Gamma \in \mathcal{L}(\mathcal{H}_N) \mid 0 \leq \Gamma \leq 1, \text{Tr}[\Gamma] = 1\}$  the set of states on the bosonic  $N$ -particle Hilbert space  $\mathcal{H}_N$  consisting of permutation symmetric, square integrable wave functions. Accordingly,  $\text{Tr}$  denotes the trace over  $\mathcal{H}_N$ . The free energy is given by

$$(3) \quad F(T, N, L) = \inf_{\Gamma \in \mathcal{S}_N} \underbrace{\{\text{Tr}[H_N \Gamma] - TS(\Gamma)\}}_{=\mathcal{F}(\Gamma)} \quad \text{with} \quad S(\Gamma) = -\text{Tr}[\Gamma \ln(\Gamma)].$$

The quantity  $S$  is called the von-Neumann entropy and the unique minimizer of the free energy functional  $\mathcal{F}$  is the Gibbs state of the system. By  $F_0(\beta, N, L)$  we denote the free energy of the ideal gas ( $v = 0$ ). We are interested in temperatures of the order of the critical temperature of the ideal gas or smaller, that is, in inverse temperatures  $\beta$  such that  $\beta \geq \text{const.} \cdot (4\pi)^{-1}((N/L^3)/\zeta(3/2))^{-2/3}$ . Here  $\zeta$  denotes the Riemann zeta function.

Apart from the above result for the trapped Bose gas in the GP limit [4], the only other known result concerning the dilute Bose gas at positive temperature concerns the free energy asymptotics in the thermodynamic limit, see [10] for the upper bound and [9] for the lower bound. We note that the second reference is a key ingredient for parts of the proof of Theorem 1 below. The first reference is not relevant for us because we give a much simpler proof for the upper bound for the free energy in the case of the GP limit. This is possible because the gas is much more dilute in this regime compared to the setting in [10]. Our main result in [5] is the following statement:

**Theorem 1:** *Assume that  $v$  is a nonnegative interaction potential with finite scattering length. Denote by  $\varrho_0(\beta, N, L)$  the expected condensate density in the canonical Gibbs state of the ideal Bose. In the combined limit  $N \rightarrow \infty$ ,  $\beta \varrho^{2/3} \geq \text{const.}$*

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

Moreover, for any sequence of states  $\Gamma_N \in \mathcal{S}_N$  with one-particle density matrices  $\gamma_N$  and

$$(5) \quad \mathcal{F}(\Gamma_N) = F_0(\beta, N, L) + 4\pi a_N L^3 \left( 2\varrho^2 - \varrho_0(\beta, N, L)^2 \right) (1 + o(1)),$$

we have

$$(6) \quad \|\gamma_N - \gamma_{N,0}\|_1 \leq o(N).$$

Here  $\gamma_{N,0}$  denotes the one-particle density matrix of the canonical Gibbs state of the ideal gas and  $\|\cdot\|_1$  is the trace norm.

We remark that the free energy in (4) has the same form as the one of the dilute Bose gas in the thermodynamic limit. The reason for this are the periodic boundary conditions. They also imply that the condensate wave function equals

a constant. The structure of the interaction term in (4) can be understood if one realizes that the exchange term in the interaction is only relevant for particles sitting in different one-particle orbitals, which is typically the case for particles in the thermal cloud but not for particles in the condensate. This is the reason why the interaction energy between particles inside the thermal cloud is twice as large as the one between particles in the condensate. The quantities related to the canonical ideal gas in Theorem 1, that is,  $F_0(\beta, N, L)$ ,  $\varrho_0(\beta, N, L)$  and  $\gamma_{N,0}$ , can be replaced by their grand canonical equivalents and the statement remains true. This is advantageous because explicit formulas are available for the latter quantities. We also remark that (6) implies BEC in the sense

$$(7) \quad \lim_{N \rightarrow \infty} \sup_{\|\phi\|=1} \frac{\langle \phi, \gamma_N \phi \rangle}{N} = \left[ 1 - \left( \frac{\beta_c}{\beta} \right)^{3/2} \right]_+,$$

where  $\beta_c$  denotes the inverse critical temperature of the ideal gas.

We conclude our discussion by highlighting two main technical novelties of our proof: The first key ingredient of our approach is a novel use of the Gibbs variational principle that goes hand in hand with the  $c$ -number substitution, which is a central technical tool in the proof in [9]. It allows us to work with a general state  $\Gamma$  instead of with a version of the grand canonical Gibbs state. Like this, we can keep the information that  $\Gamma$  has exactly  $N$  particles and we are able to quantify the coercivity of the Gibbs free energy functional  $\mathcal{F}$ . The second main novelty is a lower bound for the bosonic relative entropy of two density matrices (the difference between their free energies) in terms of a function of their trace norm difference. This bound is used in the proof of (6) and allows us to substantially simplify parts of the analysis with respect to a similar part of the proof in [4].

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