Bose-Einstein Condensation in a Dilute Trapped Gas at Positive Temperature
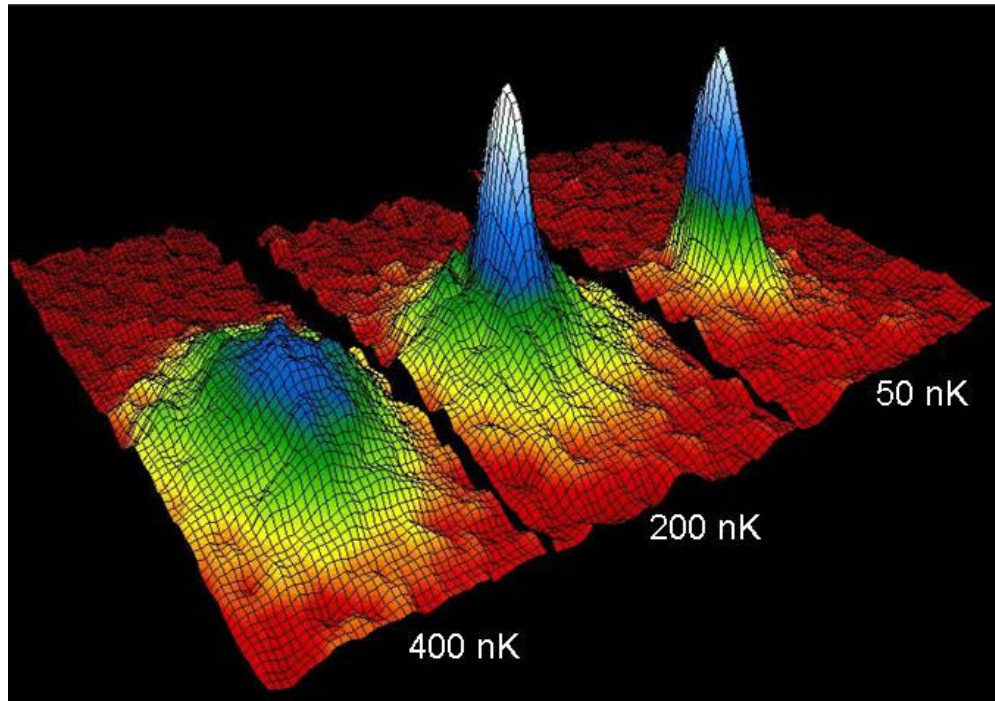
Robert Seiringer
IST Austria

Joint work with Andreas Deuchert and Jakob Yngvason
arXiv:1803.05180

Recent Results on Quantum Many-Body Systems
Herrsching, May 7–9, 2018

Introduction and Motivation

Experimental observation of **Bose-Einstein Condensation** in cold atomic gases:

In these experiments, a large number of (bosonic) atoms is confined to a trap and cooled to very low temperatures. Below a **critical temperature** condensation of a large fraction of particles into the same one-particle state occurs.

BEC was predicted by Einstein in 1924 from considerations of the **non-interacting** Bose gas. The presence of particle interactions represents a major difficulty for a rigorous derivation of this phenomenon.

The Bose Gas: A Quantum Many-Body Problem

Quantum-mechanical description in terms of the **Hamiltonian** for a gas of N bosons in a harmonic trap potential, interacting via a pair-potential $v(x)$. In appropriate units,

$$H_N = \sum_{i=1}^{N} \left(-\Delta_i + \tfrac{1}{4}\omega^2 |x_i|^2 - \tfrac{3}{2}\omega \right) + \sum_{1 \le i < j \le N} a^{-2} v(|x_i - x_j|/a)$$

As appropriate for **bosons**, H acts on $\mathcal{H}_N$, the **permutation-symmetric** wave functions $\Psi(x_1, \ldots, x_N)$ in $\bigotimes^N L^2(\mathbb{R}^3)$.

Interaction $v \ge 0$ short range, normalized to have **scattering length** equal to 1.

Gross-Pitaevskii regime of dilute gases: gap of one-particle Hamiltonian $\sim$ interaction energy per particle, i.e.,

$$\omega \sim aN\omega^{3/2} \quad , \quad a \sim \omega^{-1/2} N^{-1}$$

Dilute Bose Gases at Zero Temperature

Gross-Pitaevskii energy functional

$$\mathcal{E}^{\mathrm{GP}}(\phi) = \langle\phi| -\Delta + \tfrac{1}{4}\omega^2|x|^2 - \tfrac{3}{2}\omega|\phi\rangle + 4\pi a \int_{\mathbb{R}^3} |\phi|^4$$

with $E^{\mathrm{GP}}(N,\omega,a) = \min\{\mathcal{E}^{\mathrm{GP}}(\phi) \, : \, \int |\phi|^2 = N\} = \omega N E^{\mathrm{GP}}(1,1,Na\omega^{1/2})$.

THEOREM 1 (E.H. Lieb, R.S., J. Yngvason 2000; E.H. Lieb, R.S. 2002). *If* $Na\omega^{1/2} \to g$ *as* $N \to \infty$, *then*

$$\lim_{N\to\infty} \frac{1}{\omega N} \inf \mathrm{spec}\, H_N = E^{\mathrm{GP}}(1,1,g)$$

Moreover, for any approximate ground state Ψ_N *with one-particle density matrix* $\gamma_N = \mathrm{Tr}_{N-1}|\Psi_N\rangle\langle\Psi_N|$,

$$\lim_{N\to\infty} \big\|\gamma_N - |\varphi_g^{\mathrm{GP}}\rangle\langle\varphi_g^{\mathrm{GP}}|\big\|_1 = 0$$

The result shows in particular **complete BEC** in the GP regime at zero temperature!

The Ideal Bose Gas at Positive Temperature

In the grand-canonical ensemble,

$$N = \sum_{n \geq 0} \frac{(1+n)(1+\frac{1}{2}n)}{e^{\beta(\omega n - \mu)} - 1} = N_0 + \sum_{n \geq 1} \frac{(1+n)(1+\frac{1}{2}n)}{e^{\beta(\omega n - \mu)} - 1}$$

BEC: $N_0 \sim N$, i.e., $\beta|\mu| \sim N^{-1}$. If $|\mu| \ll \omega$ and $\beta\omega \ll 1$, one also has
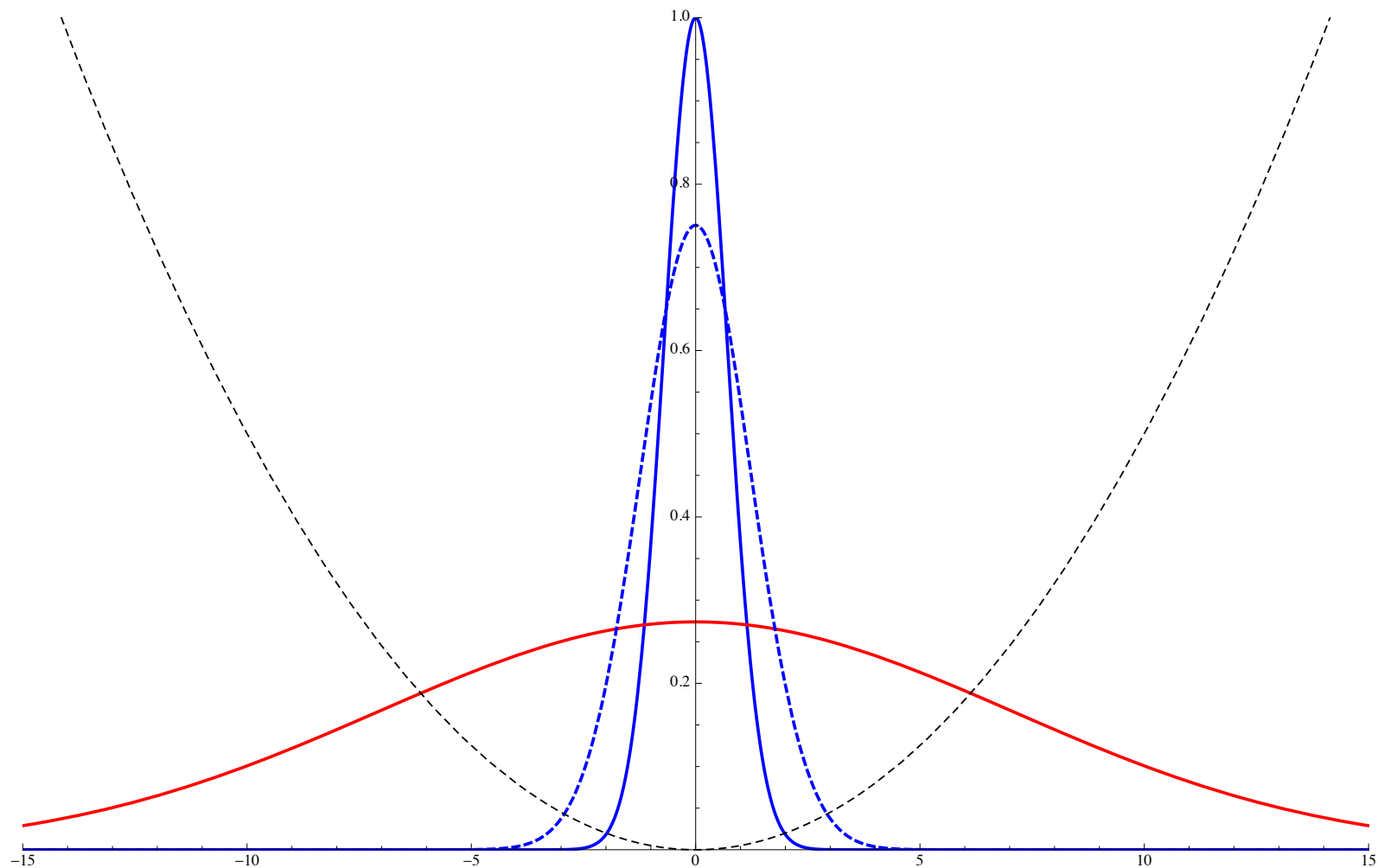
$$\sum_{n \geq 1} \frac{(1+n)(1+\frac{1}{2}n)}{e^{\beta(\omega n - \mu)}} \approx \frac{1}{2} \int_0^\infty \frac{t^2}{e^{\beta\omega t} - 1} dt = (\beta\omega)^{-3}\zeta(3)$$

This leads to the **critical temperature** $(\beta_c\omega)^{-3}\zeta(3) = N$, or

$$T_c = \omega \left(\frac{N}{\zeta(3)}\right)^{1/3}, \quad \text{and} \quad \frac{N_0}{N} \approx \left[1 - \left(\frac{T}{T_c}\right)^3\right]_+$$

in the **thermodynamic limit** (i.e., $T \sim \omega N^{1/3}$).

Separation of Length Scales

BEC: $\sim \omega^{-1/2}$, thermal cloud: $\sim \beta^{-1/2}\omega^{-1} \sim \omega^{-1/2}N^{1/6}$

THE INTERACTING GAS AT POSITIVE TEMPERATURE

Consider the **free energy**

$$F(\beta, N, \omega, a) = -\frac{1}{\beta} \ln \mathrm{Tr}_{\mathcal{H}_N} e^{-\beta H_N}$$

THEOREM 2 (A. Deuchert, R.S., J. Yngvason 2018). *As $N \to \infty$ with $T \sim \omega N^{1/3}$ and $a \sim \omega^{-1/2} N^{-1}$,*

$$\lim \frac{1}{\omega N} \left| F(\beta, N, \omega, a) - \underbrace{F_0(\beta, N, \omega)}_{O(\omega N^{4/3})} - \underbrace{E^{\mathrm{GP}}(N_0, a, \omega)}_{O(\omega N)} \right| = 0$$

Moreover, the one-particle density matrix γ of any approximate **Gibbs state** *satisfies*

$$\lim \left\| \gamma - \gamma_0 + \frac{N_0}{N} |\varphi_0\rangle\langle\varphi_0| - \frac{N_0}{N} |\varphi_g^{\mathrm{GP}}\rangle\langle\varphi_g^{\mathrm{GP}}| \right\|_1 = 0$$

with $g = N_0 a \omega^{1/2}$.

REMARKS

- **Approximate Gibbs states** are approximate minimizers of the free energy functional

$$\operatorname{Tr} H_N \Gamma - \frac{1}{\beta} S(\Gamma) \quad , \quad S(\Gamma) = -\operatorname{Tr} \Gamma \ln \Gamma$$

- Result implies **BEC** in the sense that

$$\lim \left\| \gamma - \frac{N_0}{N} |\varphi_g^{\mathrm{GP}}\rangle\langle\varphi_g^{\mathrm{GP}}| \right\|_\infty = 0$$

  with the same transition temperature and condensate fraction as the ideal gas (to leading order).

- The result is uniform in T for $T \lesssim \omega N^{1/3}$, and reproduces the earlier result as $T \to 0$.

- We work in the **canonical ensemble** but the result also holds grand-canonically.

- Generalization to other trapping potentials and dimensions (≥ 2) possible

IDEAS IN THE PROOF

Reduce to $T = 0$ problem via **spatial localization**:

Upper bound: For $\omega^{-1/2} \ll R \ll \beta^{-1/2}\omega^{-1}$,

$$\mathcal{H}_N \subset \mathcal{F}(L^2(\mathbb{R}^3)) = \mathcal{F}(L^2(B_R)) \otimes F(L^2(B_R^c))$$

choose trial state

$$|\Psi_{N_0}\rangle\langle\Psi_{N_0}\rangle \otimes \Gamma_{N-N_0}$$

with (appropriately modified) Gibbs state Γ_{N-N_0} for an ideal gas of $N - N_0$ particles confined to B_R^c, and control localization error.

Lower bound: smooth separation via **geometric localization**: given $A \geq 0$ and $B \geq 0$ in $\mathcal{B}(\mathcal{H})$ with $A^2 + B^2 = \mathbb{I}$, and Γ a state on $\mathcal{F}(\mathcal{H})$ with reduced density matrices $\gamma^{(k)}$, $\exists$ states Γ_A and Γ_B with red. density matrices $A^{\otimes k}\gamma^{(k)}A^{\otimes k}$ and $B^{\otimes k}\gamma^{(k)}B^{\otimes k}$, respectively. The entropy is subadditive, i.e., $S(\Gamma) \leq S(\Gamma_A) + S(\Gamma_B)$.

Ideas in the Proof

Control of the one-particle density matrix via a **novel coercivity estimate**:

Lemma 1. *Let*

$$S(\gamma, \sigma) = \text{Tr}_{\mathcal{H}} \left[\gamma \ln \gamma - \gamma \ln \sigma - (1 + \gamma) \ln(1 + \gamma) + (1 + \gamma) \ln(1 + \sigma) \right]$$

be the "bosonic relative entropy". Then

$$S(\gamma, \sigma) \geq C \begin{cases} \text{Tr} \left[\frac{1}{1+\sigma} \left(\frac{\gamma}{\sqrt{1+\gamma}} - \frac{\sigma}{\sqrt{1+\sigma}} \right)^2 \right] \\ \frac{[\text{Tr}(\gamma - \sigma)][^2}{\text{Tr}(\gamma + \sigma)(1 + \sigma)} \end{cases}$$

With P a (smooth) projection into B_R^c, the bounds on the free energy imply that

$$S(NP\gamma P, NP\gamma_0 P) \ll \beta \omega N$$

Together with $N\|P\gamma_0 P\|_\infty \lesssim (\beta\omega)^{-1}$ this allows to conclude the desired bound.

CONCLUSIONS

- In a combination of the **thermodynamic** and the **Gross-Pitaevskii** limit, we show that the difference between the canonical free energy of the interacting gas and the one of the noninteracting system can be obtained by minimizing the GP energy functional.

- The one-particle density matrix of any approximate minimizer of the free energy functional is to leading order given by that of the noninteracting gas but with the free **condensate wavefunction** replaced by the GP minimizer.

- There is BEC with the same transition temperature and condensate fraction as for the ideal gas (to leading order).

- Separation of length scales allows for a **spatial separation** of the condensate and the thermal cloud.

- It remains a **major open problem** to obtain results on BEC away from the GP limit, i.e., for systems that are less dilute.