Bose-Einstein condensation in a dilute, trapped gas at positive temperature

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Mathematical Physics Seminar @ Grenoble
October 15, 2018

Joint work with Robert Seiringer and Jakob Yngvason

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Goal: Prove this picture

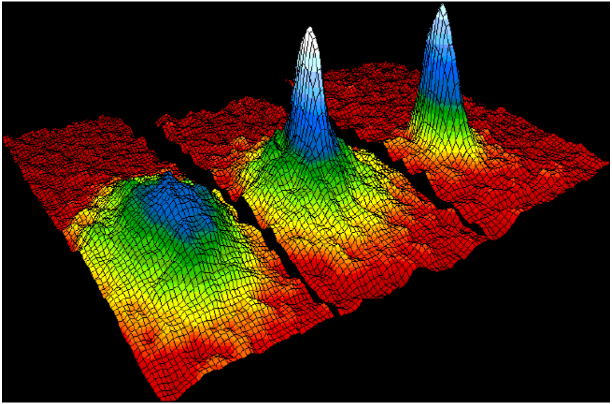


Figure: Emergence of BEC inside the thermal cloud of Rubidium atoms

Anderson et al., Observation of bose-einstein condensation in a dilute atomic vapor, Science 269, 198 (1995)

Shortest possible introduction to quantum statistical mechanics or the relevant mathematical objects

Assume we are given a Hamiltonian H_N describing N particles. To model the N–particle system related to H_N in equilibrium at temperature T, we are typically interested in:

$T = 0$	$T > 0$
Ground state (GS) Ψ_0 of H_N	Gibbs state $\frac{e^{-H_N/T}}{\mathrm{Tr}[e^{-H_N/T}]}$
GS energy $E_0 = \langle \Psi_0, H_N \Psi_0 \rangle$	Free energy $F = -T \ln \left(\mathrm{Tr} \left[e^{-H_N/T} \right] \right)$

The ideal Bose gas in the harmonic trap

The expected number of particles in the grand canonical ideal Bose gas governed by the harmonic oscillator Hamiltonian

$$h = -\Delta + \frac{\omega^2 x^2}{4} - \frac{3\omega}{2}$$

is given by

$$\overline{N} = \underbrace{\frac{1}{e^{-\beta\mu_0} - 1}}_{N_0} + \underbrace{\frac{1}{2}\sum_{n=1}^{\infty} \frac{(n+1)(n+2)}{e^{\beta(\omega n - \mu_0)} - 1}}_{N_{\mathrm{th}}}.$$

Here $\beta = T^{-1}$ denotes the inverse temperature and μ_0 is the chemical potential.

The ideal Bose gas in the harmonic trap

The expected number of particles of the grand canonical ideal Bose gas governed by the harmonic oscillator Hamiltonian

$$h = -\Delta + \frac{\omega^2 x^2}{4} - \frac{3\omega}{2}$$

is given by

$$\overline{N} \underbrace{\simeq}_{-\beta\mu_0 \ll \beta\omega \ll 1} \underbrace{\frac{1}{-\beta\mu_0}}_{N_0} + \underbrace{\frac{1}{(\beta\omega)^3} \frac{1}{2} \int_0^\infty \frac{x^2}{e^x - 1} \mathrm{d}x}_{N_{\mathrm{th}}} .$$

Here $\beta = T^{-1}$ denotes the inverse temperature and μ_0 is the chemical potential.

The thermodynamic limit in the trap

The thermodynamic limit in the harmonic trap is defined by

$$N \gg 1 \quad \text{and} \quad (\beta\omega)^{-3} \sim N.$$

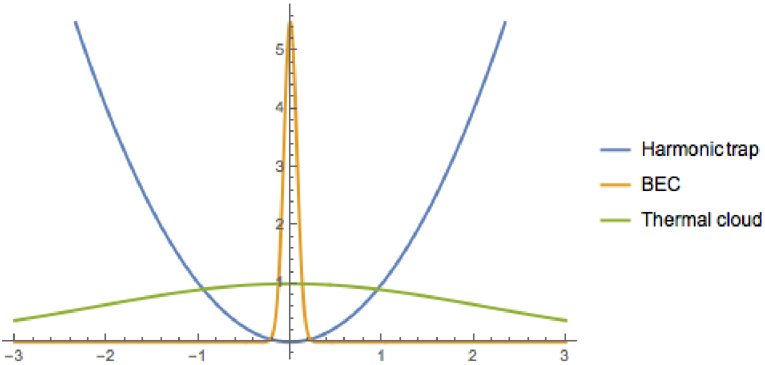
With the critical temperature

$$T_{\mathrm{c}}(N,\omega) = \omega \left(\frac{N}{\zeta(3)} \right)^{1/3},$$

the limit of the expected occupation of the ground state in the harmonic trap can be written as

$$\lim \frac{N_0(\beta,N,\omega)}{N} = \lim \left[1 - \left(\frac{T}{T_{\mathrm{c}}} \right)^3 \right]_+ .$$

Length scales



- Length scale condensate: $\omega^{-1/2}$
- Length scale thermal cloud: $\omega^{-1/2}\frac{1}{(\beta\omega)^{1/2}} \gg \omega^{-1/2}$

The model

Hamiltonian with Gross-Pitaevskii scaling:

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

with $v \geq 0$ such that scattering length is finite. The scattering length of $\omega N^2 v \left(N \omega^{1/2} x \right)$ behaves as

$$a_N \sim \omega^{-1/2} N^{-1} \quad \Rightarrow \quad a_N \ll \omega^{-1/2} \text{ and } N a_N \sim \omega^{-1/2}.$$

The free energy of the gas is given by

$$F(\beta, N, a_N, \omega) = -\tfrac{1}{\beta} \ln \left(\operatorname{Tr} \left[e^{-\beta H_N} \right] \right),$$

where the trace is taken only over symmetric functions.

GP Functional and 1-pdm

Gross-Pitaevskii (GP) functional

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

with ground state energy

$$E^{\mathrm{GP}}(N, a, \omega) = \inf_{\|\phi\|^2_{L^2(\mathbb{R}^3)} = N} \mathcal{E}^{\mathrm{GP}}(\phi)$$

and minimizer $\phi^{\mathrm{GP}}_{N,a}$. One-particle reduced density matrix (1-pdm) of state Γ_N

$$\gamma^{(1)}_N(x, y) = \mathrm{Tr}[a^*_x a_y \Gamma_N].$$

Mathematical literature on dilute Bose gases

- 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)
- Ground state asymptotics of H_N (GP limit): Lieb, Seiringer, Yngvason '00, Lieb, Seiringer '02, Boccato, Brennecke, Cenatiempo, Schlein '17
- GP limit of rotating Bose gas: Lieb, Seiringer '06, Nam, Rougerie, Seiringer '16
- Bogoliubov theory in GP scaling: Boccato, Brennecke, Cenatiempo, Schlein '18
- Dynamics governend by H_N of BEC : Erdös, Schlein, Yau '09 and '10, Pickl '15, Benedikter, de Oliveira, Schlein '15
- Free energy asymptotics of dilute Bose gas in thermodynamic limit: Seiringer '08 (Lower bound), Yin '10 (Upper bound)

Theorem: Part 1 (Asymptotics of free energy)

Assumptions:

- v is a nonnegative, radial and measurable function which is integrable outside some finite ball
- Limit: $N \to \infty$, $(\beta\omega)^{-3} \sim N$ and $a_N \sim \omega^{-1/2} N^{-1}$

Notation:

- $F(\beta, N, a_N, \omega)$ the canonical free energy related to H_N
- $F_0(\beta, N, \omega) \sim \omega N_{\mathrm{th}}^{4/3}$ the free energy of the ideal gas
- $N_0(\beta, N, \omega)$ expected number of particles in condensate of ideal Bose gas
- $E^{\mathrm{GP}}(N_0, a_N, \omega) \sim \omega N_0$ the GP energy

We have

$$\lim \frac{1}{\omega N} \left| F(\beta, N, a_N, \omega) - F_0(\beta, N, \omega) - E^{\mathrm{GP}}(N_0, a_N, \omega) \right| = 0.$$

Theorem: Part 2 (Asymptotics of 1-pdm)

- State Γ_N with 1-pdm $\gamma_N^{(1)}$ and free energy $\mathcal{F}(\Gamma_N)$
- $\gamma_{N,0}^{(1)}$ denotes 1-pdm of the non-interacting canonical Gibbs state
- φ_0 normalized ground state wavefunction of the harmonic oscillator

For any sequence of states Γ_N with

$$\lim \frac{1}{\omega N} \left| \mathcal{F}_N(\Gamma_N) - F_0(\beta, N, \omega) - E^{\mathrm{GP}}(N_0, a_N, \omega) \right| = 0$$

we have

$$\lim \frac{1}{N} \left\| \gamma_N^{(1)} - \left(\gamma_{N,0}^{(1)} - N_0 |\varphi_0\rangle\langle\varphi_0| + |\phi^{\mathrm{GP}}_{N_0,a_N}\rangle\langle\phi^{\mathrm{GP}}_{N_0,a_N}| \right) \right\|_1 = 0.$$

Remarks

- The result for 1-pdm implies BEC in the form

$$\lim \frac{1}{N} \left\| \gamma_N^{(1)} - |\phi^{\mathrm{GP}}_{N_0,a_N}\rangle\langle\phi^{\mathrm{GP}}_{N_0,a_N}| \right\| = 0$$

- Extension to non-isotropic harmonic trap possible
- Extension to radial potentials going as $|x|^\alpha$ for $|x| \to \infty$ with $0 < \alpha < \infty$ possible
- All quantities (interacting and non-interacting) can be replaced by grand-canonical versions
- Uniformity in temperature as long as $T \leq CT_{\mathrm{c}}$ for some $C > 0$
- Extension to $d = 2$ with natural replacements possible

And now some ideas of the proof...

Proof of lower bound: Gibbs variational principle

Denote by $\mathcal{S}_N$ the set of all N-particle states:

$$\mathcal{S}_N = \left\{ \Gamma \in \mathcal{L}\left(L^2\left(\mathbb{R}^{3N}\right)\right) \;\middle|\; 0 \leq \Gamma \leq 1, \operatorname{Tr}[\Gamma] = 1, \operatorname{Tr}[H_N \Gamma] < \infty \right\}.$$

The free energy can be characterized via the Gibbs variational principle:

$$F(\beta, N, \omega) = \min_{\Gamma \in \mathcal{S}_N} \left\{ \operatorname{Tr}[H_N \Gamma] - \tfrac{1}{\beta} S(\Gamma) \right\},$$

where the entropy $S(\Gamma)$ is given by

$$S(\Gamma) = -\operatorname{Tr}[\Gamma \ln(\Gamma)].$$

Proof of lower bound: IMS localization formula

Let $j_1, j_2 \in C^\infty(\mathbb{R}^3)$ be a partition of unity in the sense that

$$j_1(x)^2 + j_2(x)^2 = 1 \quad \text{for all } x \in \mathbb{R}^3.$$

Then

$$-\Delta = -j_1(x)\Delta j_1(x) - j_2(x)\Delta j_2(x) - (\nabla j_1(x))^2 - (\nabla j_2(x))^2 .$$

Let $\omega^{-1/2} \ll R \ll \omega^{-1/2}(\beta\omega)^{-1/2}$ and choose j_1, j_2 such that

$$\text{supp}(j_1) \approx B(R) \quad \text{and} \quad \text{supp}(j_2) \approx B(R)^c.$$

We can write the energy of a state Γ as:

$$\text{Tr}\,[H_N \Gamma] \geq \text{Tr}\,(h j_1 \gamma_\Gamma j_1) + \text{Tr}\,(h j_2 \gamma_\Gamma j_2) + \text{Tr}\left(V j_1^{\otimes 2} \gamma_\Gamma^{(2)} j_1^{\otimes 2}\right)$$
$$- \text{localization error.}$$

Proof of lower bound: geometric localization in Fock space

Lemma

Let Γ be a state on $\mathcal{F}(\mathcal{H})$ (Fock space) with k-particle density matrices $\gamma_\Gamma^{(k)}$, $k \geq 1$ and let j_1, j_2 as above.

Then there exist unique states Γ_{j_1} and Γ_{j_2} on $\mathcal{F}(\mathcal{H})$ with k-particle density matrices $j_1^{\otimes k} \gamma_\Gamma^{(k)} j_1^{\otimes k}$ and $j_2^{\otimes k} \gamma_\Gamma^{(k)} j_2^{\otimes k}$, respectively. Moreover, the entropies of these states are related by

$$S(\Gamma) \leq S(\Gamma_{j_1}) + S(\Gamma_{j_2}).$$

Proof of lower bound: Minimization

By $\mu^{\mathrm{GP}}(N_0)$ we denote the GP chemical potential. Using the Lemma, the free energy of the state Γ can be written as:

$$\begin{aligned}\mathrm{Tr}\,(H_N\Gamma) - TS(\Gamma) \geq\, & \mathrm{Tr}\left[\left(H - \mu^{\mathrm{GP}}(N_0)\hat{N}\right)\Gamma_{j_1}\right] - TS\left(\Gamma_{j_1}\right) \\ & + \mathrm{Tr}\left[\left(H_0 - \mu^{\mathrm{GP}}(N_0)\hat{N}\right)\Gamma_{j_2}\right] - TS\left(\Gamma_{j_2}\right) \\ & + \mu^{\mathrm{GP}}(N_0)N - \text{localization error.}\end{aligned}$$

This allows us to minimize over Γ_{j_1} and Γ_{j_2} separately.

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

Proof of asymptotics of 1-pdm: Starting point

Let Γ_N be a sequence of states such that

$$\operatorname{Tr}\left[H_N \Gamma_N\right] - TS(\Gamma_N) = F_0(\beta, N, \omega) + E^{\mathrm{GP}}(N_0, a_N, \omega) + o(\omega N)$$

as N tends to infinity. We then have

$$o(\omega N) \geq \operatorname{Tr}\left[\left(H^{\mathrm{D}}_{\leq R} - \mu^{\mathrm{GP}} \hat{N}\right) \Gamma_{N,j_1}\right] - E^{\mathrm{GP}}(N_0, a_N, \omega) + \mu^{\mathrm{GP}} N_0$$

as well as

$$o(\omega N) \geq \operatorname{Tr}\left[\left(H^{0,\mathrm{D}}_{\geq R} - \mu^{\mathrm{GP}} \hat{N}\right) \Gamma_{N,j_2}\right] - TS\left(\Gamma_{N,j_2}\right) \\ - F_0(\beta, N, \omega) + \mu^{\mathrm{GP}} N_{\mathrm{th}}.$$

Proof of asymptotics of 1-pdm: Relative entropy

Let $\varphi : [0,1] \to \mathbb{R}$ be given by

$$\varphi(x) = x \ln(x) - (1+x) \ln(1+x).$$

For two trace-class operators γ, γ_0 with $0 \leq \gamma, \gamma_0$ the relative entropy of γ with respect to γ_0 is defined to be

$$\mathcal{S}\left(\gamma, \gamma_0\right) = \mathrm{Tr}\left[\varphi(\gamma) - \varphi(\gamma_0) - \varphi'(\gamma_0)\left(\gamma - \gamma_0\right)\right].$$

The lower bound implies

$$o(\omega N) \geq \tfrac{1}{\beta} \mathcal{S}\left(j_2 \gamma_N j_2, \tilde{\gamma}_0^{\mathrm{gc}}\right),$$

where $\tilde{\gamma}_0^{\mathrm{gc}}$ is a slightly modified version of γ_0^{gc} without a condensate.

Proof of asymptotics of 1-pdm: Lower bound for relative entropy

Lemma

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

$$\mathcal{S}(\gamma, \gamma_0) \geq C \operatorname{Tr} \left(\frac{1}{1+\gamma_0} \left(\frac{\gamma}{\sqrt{1+\gamma}} - \frac{\gamma_0}{\sqrt{1+\gamma_0}} \right)^2 \right)$$

and

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

Proof of asymptotics of 1-pdm: Conclusion from the Lemma

Let $j_2 \gamma_N j_2$ and $\tilde{\gamma}_0^{\mathrm{gc}}$ be given as above. The bound

$$o(\omega N) \geq \frac{1}{\beta} \mathcal{S}\left(j_2 \gamma_N j_2, \tilde{\gamma}_0^{\mathrm{gc}}\right)$$

together with the Lemma from the previous slide implies

$$\lim \frac{1}{N} \left\| j_2 \gamma_N j_2 - \tilde{\gamma}_0^{\mathrm{gc}} \right\|_1 = 0.$$

Note that the free energy of $j_2 \gamma_N j_2$ and the one of $\tilde{\gamma}_0^{\mathrm{gc}}$ are of order $\omega N^{4/3}$.

Proof of asymptotics of 1-pdm: Final steps

What we have:

$$j_1 \gamma_N j_1 \simeq |\phi^{\mathrm{GP}}_{N_0,a_N}\rangle\langle\phi^{\mathrm{GP}}_{N_0,a_N}| \quad \textit{and} \quad j_2 \gamma_N j_2 \simeq \gamma_0^{gc} - N_0 |\varphi_0\rangle\langle\varphi_0|.$$

It remains to

- get rid of the localization functions j_1 and j_2,
- estimate the off-diagonal contributions $\|j_1 \gamma_N j_2\|_1$ and $\|j_2 \gamma_N j_1\|$,
- show that the canonical and the grand canonical 1-pdms are close.

Thank you for your attention!

Proof of lower bound: Relation between canonical and grand canonical quantities

Lemma

Assume the chemical potential μ is such that the expected number of particles $\overline{N}$ in the grand canonical ensemble is an integer. Then

$$F_{\mathrm{c}}(\overline{N}) \geq F_{\mathrm{gc}}(\mu) \geq F_{\mathrm{c}}(\overline{N}) - \ln(1+\overline{N}) - 1.$$

Additionally, we have

$$|N_0 - N_0^{\mathrm{gc}}| \leq \|\gamma_0^{\mathrm{gc}} - \gamma_0^{\mathrm{c}}\|_1 \lesssim N^{1/2}\left(\ln(N)\right)^{1/2} + N^{1/3}\ln(N)\,.$$