

An effective equation to study Bose gases at all densities

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Grazie, Giovanni!
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Bose-Einstein condensation

- System of many Bosons, e.g. Helium atoms, Rubidium atoms, etc...
- Bose-Einstein condensate: most particles are in the same quantum state.
- Predicted theoretically in 1924-1925, experimentally observed in 1995.
- Mathematical understanding: still no proof of the existence of a condensate (at finite density, in the presence of interactions and in the continuum).

Repulsive Bose gas

- Potential: $v(r) \geq 0$ and $v \in L_1(\mathbb{R}^3)$, Hamiltonian on a torus of volume V :

$$H_N := -\frac{1}{2} \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} v(|x_i - x_j|)$$

- Ground state: ψ_0 , energy E_0 .
- Observables in the **thermodynamic limit**: ground state energy per particle and condensate fraction: P_i : projection onto condensate state

$$e_0 := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{E_0}{N}, \quad \eta_0 := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{1}{N} \sum_{i=1}^N \langle \psi_0 | P_i | \psi_0 \rangle.$$

Low density

- Bogolyubov theory: **approximation scheme** that reduces the problem to an effective **1-particle problem**.
- Predictions [Lee, Huang, Yang, 1957]:

- ▶ Energy:

$$e_0 = 2\pi\rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right)$$

- ▶ Condensate fraction:

$$1 - \eta_0 \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

Low density

- Energy asymptotics: **proved**: [Lieb, Yngvason, 1998], [Yau, Yin, 2009], [Fournais, Solovej, 2020], [Basti, Cenatiempo, Schlein, 2021].
- Condensate fraction: **still open** in the thermodynamic limit (there are proofs of condensation in the Gross-Pitaevskii regime (ultra-dilute): [Lieb, Seiringer, 2002], [Bocato, Brennecke, Cenatiempo, Schlein, 2018]).

High density

- [Bogolyubov, 1947]: if $\hat{v} \geq 0$.

$$e_0 \sim \frac{\rho}{2} \int v$$

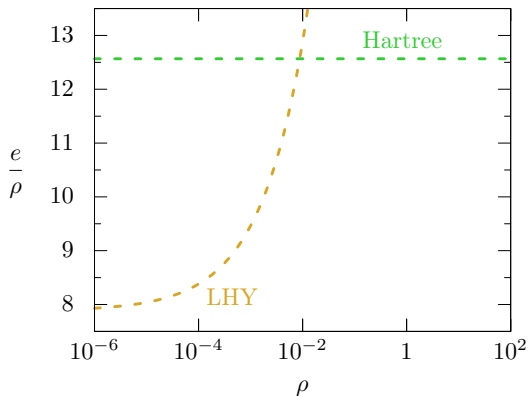
Hartree (mean field) energy.

- Proved in [Lieb, 1963].
- Condensate fraction (open problem):

$$\eta \rightarrow 1$$

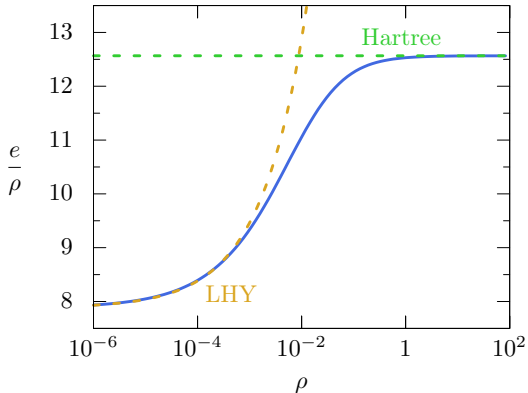
Energy as a function of density

For $v(x) = e^{-|x|}$:



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Derivation of the equation

- [Lieb, 1963].
- Integrate $H_N\psi_0 = E_0\psi_0$:

$$\int dx_1 \cdots dx_N \left(-\frac{1}{2} \sum_{i=1}^N \Delta_i \psi_0 + \sum_{1 \leq i < j \leq N} v(x_i - x_j) \psi_0 \right) = E_0 \int dx_1 \cdots dx_N \psi_0$$

- Therefore,

$$\frac{N(N-1)}{2} \int dx_1 dx_2 v(x_1 - x_2) \frac{\int dx_3 \cdots dx_N \psi_0}{\int dx_1 \cdots dx_N \psi_0} = E_0$$

Derivation of the equation

- $\psi_0 \geq 0$, so it can be thought of as a probability distribution.
- g_n : **correlation functions** of $V^{-N}\psi_0$

$$g_n(x_1, \dots, x_n) := \frac{V^n \int dx_{n+1} \cdots dx_N \psi_0(x_1, \dots, x_N)}{\int dx_1 \cdots dx_N \psi_0(x_1, \dots, x_N)}$$

- Thus,

$$\frac{E_0}{N} = \frac{N-1}{2V} \int dx v(x) g_2(0, x)$$

Hierarchy

- Equation for g_2 : integrate $H_N\psi_0 = E_0\psi_0$ with respect to x_3, \dots, x_N :

$$-\frac{1}{2}(\Delta_x + \Delta_y)g_2(x, y) + \frac{N-2}{V} \int dz (v(x-z) + v(y-z))g_3(x, y, z) \\ + v(x-y)g_2(x, y) + \frac{(N-2)(N-3)}{2V^2} \int dz dt v(z-t)g_4(x, y, z, t) = E_0g_2(x, y)$$

- Factorization **assumption**:

$$g_3(x_1, x_2, x_3) = g_2(x_1, x_2)g_2(x_1, x_3)g_2(x_2, x_3)$$

$$g_4(x_1, x_2, x_3, x_4) = \prod_{i < j} (g_2(x_i, x_j) + O(V^{-1}))$$

Big equation

- In the thermodynamic limit, if $u(x) := 1 - g_2(0, x)$,

$$-\Delta u(x) = (1 - u(x)) (v(x) - 2\rho K(x) + \rho^2 L(x))$$

$$K := u * S, \quad S(y) := (1 - u(y))v(y)$$

$$L := u * u * S - 2u * (u(u * S)) + \frac{1}{2} \int dydz u(y)u(z-x)u(z)u(y-x)S(z-y).$$

- “Big” equation:

$$L \approx u * u * S - 2u * (u(u * S))$$

Simple equation

- Further approximate $S(x) \approx \frac{2e}{\rho} \delta(x)$ and $u \ll 1$.
- Simple equation

$$-\Delta u(x) = (1 - u(x))v(x) - 4eu(x) + 2e\rho u * u(x)$$

$$e = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

- **Theorem 1:** If $v(x) \geq 0$ and $v \in L_1 \cap L_2(\mathbb{R}^3)$, then the simple equation has an integrable solution (proved constructively), with $0 \leq u \leq 1$.

Energy for the simple equation

- **Theorem 2:**

$$\frac{e}{\rho} \xrightarrow{\rho \rightarrow \infty} \frac{1}{2} \int dx v(x)$$

(note that there is no condition that $\hat{v} \geq 0$). This coincides with the **Hartree energy**.

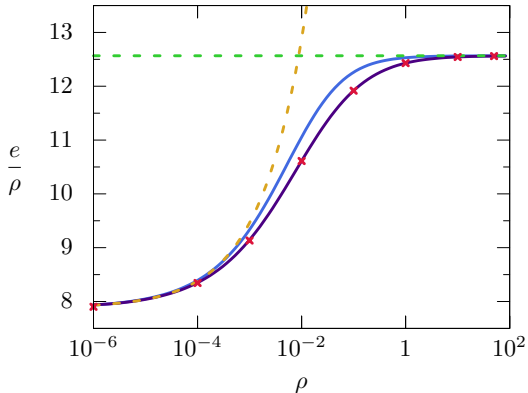
- **Theorem 3:**

$$e = 2\pi\rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right)$$

This coincides with the **Lee-Huang-Yang prediction**.

Energy

$v(x) = e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Condensate fraction

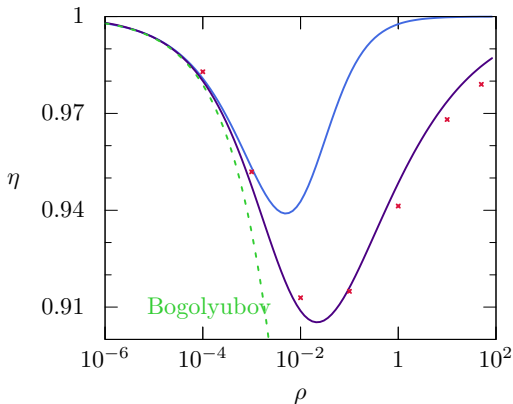
- **Theorem 4:** For the [simple equation](#), as $\rho \rightarrow 0$

$$1 - \eta \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

which coincides with [Bogolyubov's prediction](#).

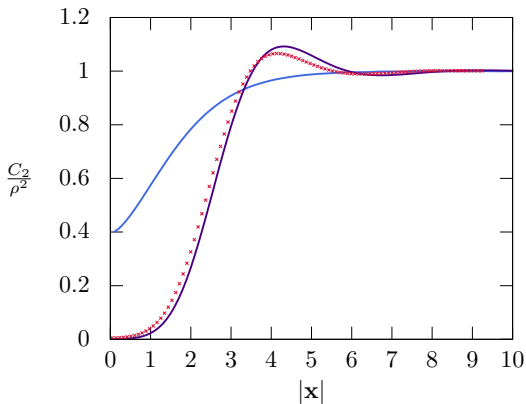
Condensate fraction

$v(x) = e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Two point correlation function

$v(x) = 16e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Summary and outlook

- Two **effective equations**: the **big equation** and the **simple equation**, which are **non-linear 1-particle equations**.
- Reproduce the known results for both **small and large densities**.
- Their derivation is **different from Bogolyubov theory**, so they may give new insights onto studying the Bose gas in these asymptotic regimes.
- The **big equation** is **quantitatively accurate** at intermediate densities.
- This opens up the possibility of studying the physics of the **Bose gas at intermediate densities**.

Open problems

- LHY as an **upper bound** at low density using the **simple equation** to construct an Ansatz.
- **Uniqueness** of the solution of the **simple equation** (done for small and large ρ).
- **Existence** (and uniqueness) of the solution of the **big equation**.
- Bosons in a **trap**.

Upper bound at low density

- [Yau, Yin, 2009]: proof for **weak, smooth**, rapidly decaying potentials.
- [Basti, Cenatiempo, Schlein, 2021]: extended for L_3 (and compactly supported) potentials (excludes hard-core interactions).
- **Simple Equation**: our analysis holds for the hard-core, so if one could find a good **Ansatz** from it, one might get an upper bound for the energy in this case.
- Idea for Ansatz? (Jastrow, Dyson-Jastrow?).

Upper bound at low density: Jastrow function

- Idea:

$$\psi = \prod_{i < j} e^{-u(x_i - x_j)}$$

- Why this: $\rho \ll 1$, and if $\rho \|u\|_1 \ll 1$,

$$g_2 \sim 1 - u.$$

- Again, if $\rho \|u\|_1 \ll 1$, we would be able to compute the energy of ψ using a cluster expansion!
- However, $\|u\|_1 = \frac{1}{\rho}$!

The uniqueness problem

$$-\Delta u(x) = (1 - u(x))v(x) - 4eu(x) + 2e\rho u * u(x), \quad e = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

- Change the point of view: **fix** $e > 0$, and compute ρ and u .
- **Iteration:** $u_0 = 0$,

$$(-\Delta + 4e + v)u_n = v + 2e\rho_{n-1}u_{n-1} * u_{n-1}, \quad \rho_n := \frac{2e}{\int dx (1 - u_n(x))v(x)}.$$

The uniqueness problem

- **Lemma:** $u_n(x)$ is an **increasing** sequence, and is **bounded** $u_n(x) \leq 1$. It converges to a function u , which is the **unique** integrable solution of the equation **with e fixed**.
- **Lemma:** $e \mapsto \rho(e)$ is **continuous**, and $\rho(0) = 0$ and $\rho(\infty) = \infty$, which allows us to compute solutions for the problem at fixed ρ .
- We thus have a **restricted** notion of uniqueness. The full uniqueness would follow from a proof that $e \mapsto \rho(r)$ is **monotone increasing** (which must be true for the physics to make sense).

Existence for the Big Equation

- Numerical method: **Newton algorithm**.
- For the existence of a solution, it would suffice to prove that the Newton algorithm has a **Basin of attraction**. (Kantorovich-like theorem?)
- Such a result, applied to the **Simple Equation**, would imply the **uniqueness** of a solution (provided we have convergence in an appropriate norm).