

# An effective equation to study Bose gasses at all densities

Ian Jauslin

joint with **Eric A. Carlen**, **Markus Holzmann**, **Elliott H. Lieb**

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<http://ian.jauslin.org>

# Bose-Einstein condensation

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- System of many Bosons, e.g. **Helium** atoms, **Rubidium** atoms, etc...
- **Bose-Einstein condensate**: most particles are in the same quantum state.
- Related to the phenomena of **superfluidity** (flow with zero viscosity) and **superconductivity** (currents with zero resistance).
- 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

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- Potential:  $v(r) \geq 0$  and  $v \in L_1(\mathbb{R}^3)$ , Hamiltonian:

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

- Ground state:  $\psi_0$ , 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

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- 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

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

## High density

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

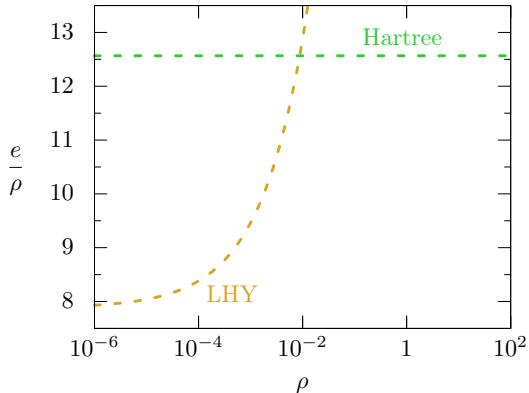
$$e_0 \sim \frac{\rho}{2} \int v$$

- **Proved** in [Lieb, 1963].
- The ultra-concentrated limit is the **Hartree** regime. [Seiringer, 2011].

# Energy as a function of density

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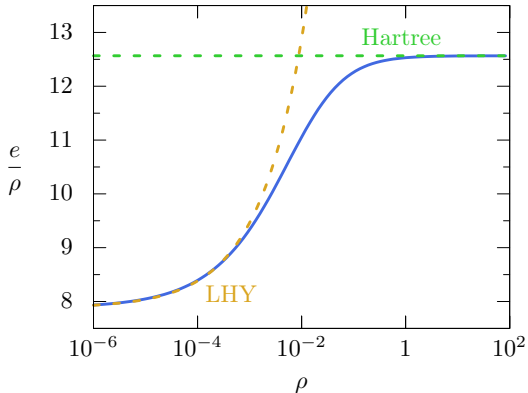
For  $v(x) = e^{-|x|}$ :



# Energy as a function of density

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





## Derivation of the equation

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- [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

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- Thus,

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

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

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

## Hierarchy

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- 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

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

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

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

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

- “Big” equation:

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

## Simple equation

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- 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

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- **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:**

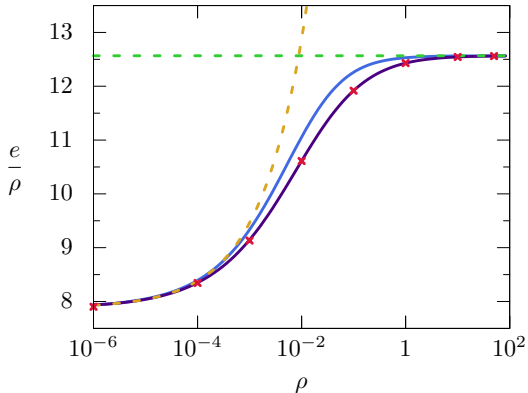
$$e = 2\pi\rho a \left( 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right)$$

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

# Energy

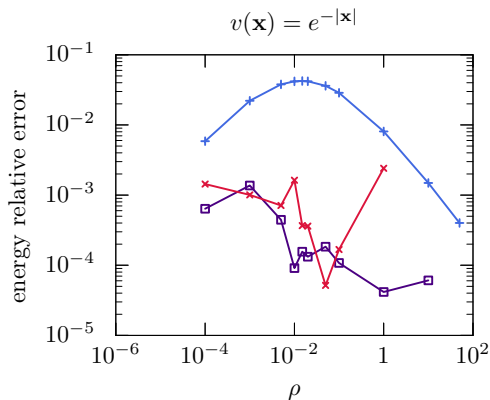
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$v(x) = e^{-|x|}$ , Blue: simple equation; purple: big equation; red: Monte Carlo



# Energy

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





## Condensate fraction

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- Add a parameter  $\mu$  to the Hamiltonian:

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

- Projection onto condensate wavefunction:  $P_i$ .
- Condensate fraction:

$$\eta_0 := \frac{1}{N} \langle \psi_0 | \sum_{i=1}^N P_i | \psi_0 \rangle = -\frac{1}{N} \partial_\mu \langle \psi_0 | H_N(\mu) | \psi_0 \rangle |_{\mu=0} \equiv -\partial_\mu e_0(\mu) |_{\mu=0}$$

## Condensate fraction

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

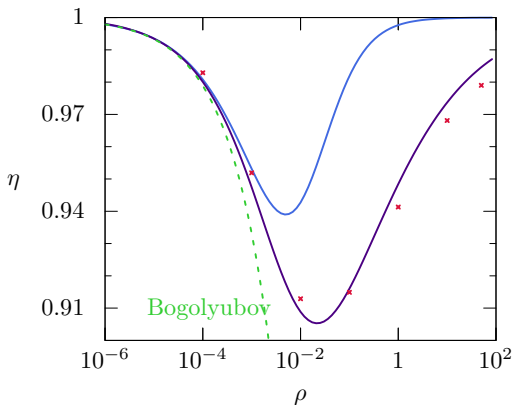
$$1 - \eta \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

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

## Condensate fraction

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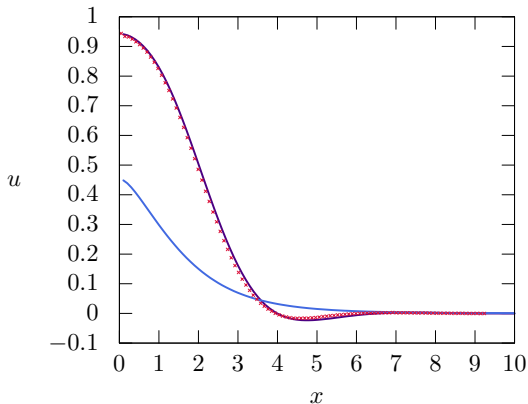
$v(x) = e^{-|x|}$ , Blue: simple equation; purple: big equation; red: Monte Carlo



# Linear correlation function

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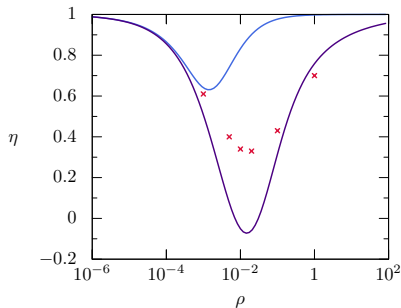
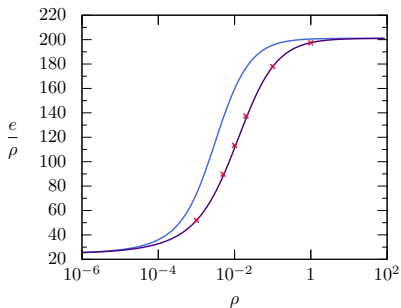
$v(x) = 16e^{-|x|}$ , Blue: simple equation; purple: big equation; red: Jastrow



# Limitations of the simple and big equations

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- Only works at high densities for  $\hat{v} \geq 0$ .
- Less accurate for **large potentials**: for  $v(x) = 16e^{-|x|}$ ,



## Conclusions and outlooks

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- 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

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- Analysis of the **simple equation**: **Monotonicity** of  $e(\rho)$ , and **convexity** of  $\rho e(\rho)$ . (So far, we have proofs for small and large  $\rho$ ). Similarly, prove that  $0 \leq \eta \leq 1$ . (We have a proof for small  $\rho$ .)
- Analysis of the **big equation**: everything is still open.
- Relate these equations back to the **many-body Bose gas**.