

# The Simplified approach to the Bose gas

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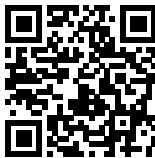
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arXiv: 2308.00290



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# Motivation

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- Effective theories to study interacting Bose gases: Bogolyubov, Gross-Pitaevskii, Hartree, etc...
- Many successes, but still many open problems, especially in the thermodynamic limit (superfluidity, Bose-Einstein condensation, etc...).
- The Simplified approach [Lieb, 1963]: single-particle non-linear effective equation(s) to study the ground state properties of repulsive Bose gases.
  - ▶ Reproduces known and conjectured results at low and high density.
  - ▶ Makes physical predictions (good agreement with Monte-Carlo) at intermediate densities.

# Repulsive Bose gas

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- Potential:  $v(r) \geq 0$ ,  $\hat{v} \geq 0$  and  $v \in L_1(\mathbb{R}^3)$ , 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 (**zero temperature**):  $\psi_0$ , energy  $E_0$ .
- Observables in the **thermodynamic limit**: for instance, ground state energy per particle

$$e_0 := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{E_0}{N}.$$

## The Simplified approach

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- [Lieb, 1963], [Jauslin, 2025].
- 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,

$$\frac{N(N-1)}{2} \int dx_1 dx_2 v(x_1 - x_2) \frac{\int dx_3 \cdots dx_N \psi_0(x)}{\int dy_1 \cdots dy_N \psi_0(y)} = E_0$$

## The Simplified approach

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

$$g_n(x_1, \dots, x_n) := \frac{V^n \int dx_{n+1} \cdots dx_N \psi_0(x_1, \dots, x_N)}{\int dy_1 \cdots dy_N \psi_0(y_1, \dots, y_N)}$$

- Thus,

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

## Hierarchy

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

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

- **Infinite hierarchy** of equations.

## Factorization assumption

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- **Factorization assumption:** for  $n = 3, 4$ ,

$$g_n(x_1, \dots, x_n) = \prod_{1 \leq i < j \leq n} (1 - u_n(x_i - x_j)), \quad u_n \in L_1(\mathbb{R}^3)$$

- Consistency condition:

$$\int \frac{dx_3}{V} g_3(x_1, x_2, x_3) = g_2(x_1, x_2), \quad \int \frac{dx_3}{V} \frac{dx_4}{V} g_4(x_1, x_2, x_3, x_4) = g_2(x_1, x_2)$$

- Remark: the factorization assumption **cannot hold exactly:**

$$\int \frac{dx_4}{V} g_4(x_1, x_2, x_3, x_4) \neq g_3(x_1, x_2, x_3)$$

## Big equation

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

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

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

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

- “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:** If  $v(x) \geq 0$  and  $v \in L_1 \cap L_{\frac{3}{2}+\epsilon}(\mathbb{R}^3)$ , then the simple equation has an integrable solution (proved constructively), with  $0 \leq u \leq 1$ .

## Comparison to the many-body Bose gas: notation

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- Ground state energy per particle:
  - ▶ Many-body Bose gas:  $e_0$
  - ▶ Simplified approach:  $e_s$
- In general, for a quantity  $A$ :
  - ▶ Many-body Bose gas:  $A_0$
  - ▶ Simplified approach:  $A_s$

## The Ground state energy

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- **Theorem:** [Bogolyubov, 1947], [Lee, Huang, Yang, 1957] [Lieb, Yngvason, 1998], [Yau, Yin, 2009], [Fournais, Solovej, 2020], [Basti, Cenatiempo, Schlein, 2021]. At **low density**,

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

- **Theorem:** For the **Simple equation**, at **low density**

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

# The Ground state energy

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- **Theorem:** [Lieb, 1963]. At **high density**,

$$\frac{e_0}{\rho} \xrightarrow{\rho \rightarrow \infty} \frac{1}{2} \int dx v(x)$$

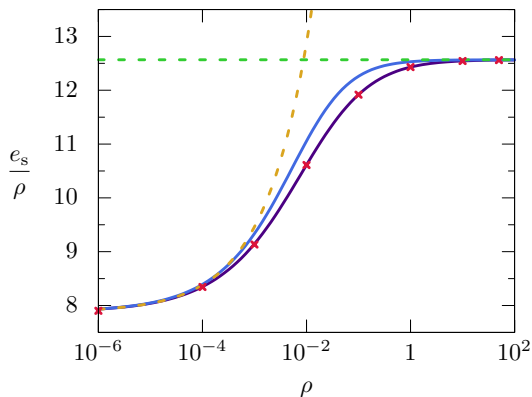
- **Theorem:** For the **Simple equation**, at **high density**

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

# The Ground state energy

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For  $v(x) = e^{-|x|}$ : Simple equation, Big equation, LHY, Hartree, Monte Carlo



## Condensate fraction

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- Let  $P_i$  be the projector onto the constant state  $V^{-\frac{1}{2}}$  for the  $i$ -th particle,

$$\eta_0 := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{1}{N} \sum_i \langle \psi_0 | P_i | \psi_0 \rangle$$

- **Conjecture:** [Lee, Huang, Yang, 1957] At **low density**,

$$\eta_0 = 1 - \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}} + o(\sqrt{\rho a^3})$$

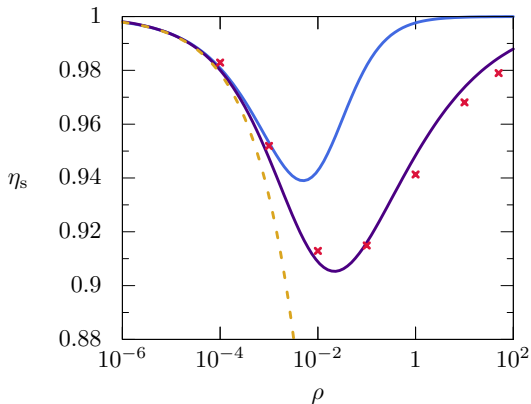
- **Theorem:** For the **Simple equation**, if  $(1 + |x|^4)v \in L_1 \cap L_2$ , then

$$\eta_s = 1 - \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}} + o(\sqrt{\rho a^3})$$

## Condensate fraction

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For  $v(x) = e^{-|x|}$ : Simple equation, Big equation, Bogolyubov, Monte Carlo



## Two-point correlation

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$$C_0^{(2)}(y-z) := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \sum_{i,j} \langle \psi_0 | \delta(y-x_i) \delta(z-x_j) | \psi_0 \rangle.$$

• **Conjecture:** [Lee, Huang, Yang, 1957] As  $\sqrt{\rho a}|x| \rightarrow \infty$ ,

$$\frac{1}{\rho^2} C_0^{(2)}(x) - 1 \sim \frac{\frac{16a}{\pi^3 \rho}}{|x|^4}$$

• **Theorem:** For the [Simple equation](#), if  $(1 + |x|^6)v \in L_1$ , then

$$\frac{1}{\rho^2} C_s^{(2)}(x) - 1 \sim \frac{c(\rho)}{|x|^4} + r(x)$$

with  $|x|^4 r \in L_2 \cap L_\infty$ .

## Universal Tan relations

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- **Momentum distribution:** if  $K_i(k)$  is the projector on  $e^{ikx}$  for  $i$ ,

$$\mathcal{M}_0(k) := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{1}{N} \sum_{i=1}^N \langle \psi_0 | K_i(k) | \psi_0 \rangle$$

- **Conjecture:** (Bogolyubov) as  $\rho \rightarrow 0$  with  $\kappa := |k|/(2\sqrt{2\pi\rho a})$  fixed,

$$\mathcal{M}_0(k) \sim \frac{1}{2\rho} \left( \frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} - 1 \right)$$

- **Theorem:** For the **Simple equation**, as  $\rho \rightarrow 0$  with  $\kappa := |k|/(2\sqrt{e})$  fixed,

$$\mathcal{M}_s(k) \sim \frac{1}{2\rho} \left( \frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} - 1 \right)$$

## Universal Tan relations

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- If one takes the limit  $\kappa \rightarrow \infty$  after  $\rho \rightarrow 0$ , we get the **Universal Tan relation** [Tan, 2008] [Combescot, Alzetto, Leyronas, 2009]

$$\mathcal{M}_0(k) \sim \frac{16\pi^2 \rho a^2}{|k|^4}$$

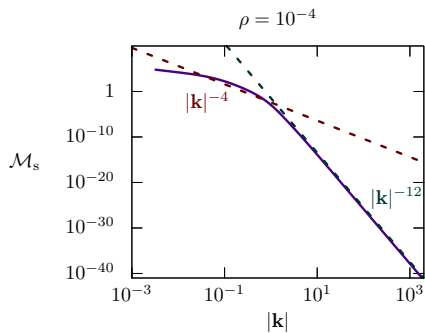
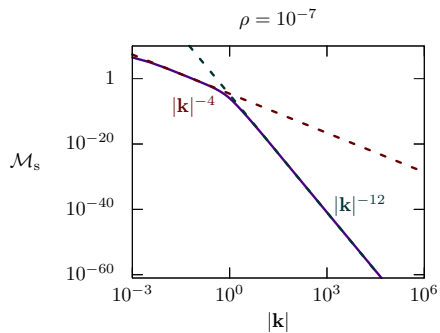
- The **Simple equation** predicts that the Tan relation holds **in the regime**

$$\sqrt{\rho a} \ll |k| \ll 1$$

and so it predicts that the Tan relations will break down at intermediate densities.

# Breakdown of the Universal Tan relations

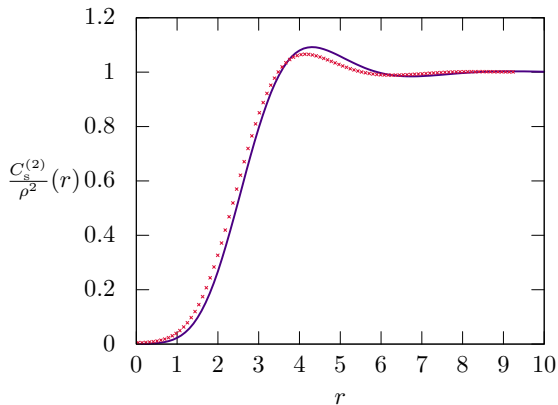
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# Two-point correlation function at intermediate density

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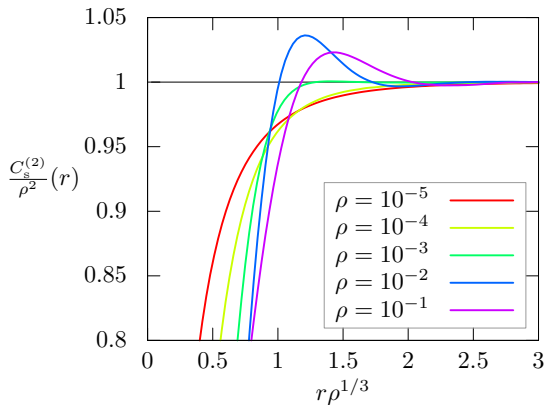
$v(x) = 16e^{-|x|}$ ,  $\rho = 0.02$  Big equation, Monte Carlo



# Two-point correlation function at intermediate density

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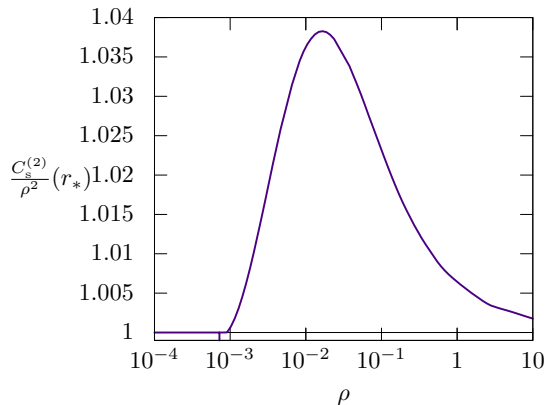
$$v(x) = 8e^{-|x|}, \rho = 10^{-5}-10^{-1}$$



## Two-point correlation function at intermediate density

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$v(x) = 8e^{-|x|}$ , maximal value as a function of  $\rho$ :



## “Liquid” behavior

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- Correlation function:
  - ▶ Maximum above 1: there is a length scale at which it is **more probable** to find pairs of particles.
  - ▶ **No** long range order: **Short-range order**.

## Summary

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- The **Simplified approach** is based on an **uncontrolled approximation**, nevertheless, it reproduces known and conjectured results for
  - ▶ the **energy** at low and high density,
  - ▶ the **condensate fraction** at low density,
  - ▶ the **two-point correlation function** at low density,
  - ▶ the **Universal Tan relations** at low density.
- It also appears to be **quantitatively accurate at all densities** (for some potentials), and predicts a non-trivial, “**liquid**”-like behavior at **intermediate densities**, as well as a breakdown of the Universal Tan relations.

# Open problems

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- **Mathematics:**

- ▶ **Uniqueness** of solutions for the **Simple equation**.
- ▶ **Existence** of solutions for the **Big equation**.
- ▶ **Positivity** of the prediction for the condensate fraction.
- ▶ **Variational formulation** of the **Simple equation**.

- **Physics:**

- ▶ Further investigation of the **intermediate density regime**.
- ▶ Extension to **positive temperature**.
- ▶ Add a **trapping potential** and connect to Gross-Pitaevskii theory.

# Open problems

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- **Mathematical Physics**

- ▶ **Control** the factorization assumption.
- ▶ Construct a **trial state** for the many-body Bose gas. Natural choice: factorized wavefunction function

$$\psi(x_1, \dots, x_N) = \prod_{i < j} e^{-u(x_i - x_j)}$$

where  $u$  is the solution to the **Simple equation**.