

# Non-perturbative behavior of interacting Bosons at intermediate densities

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# Bosons

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- Quantum particles are either **Fermions** or **Bosons** (in 3D).
- Fermions: electrons, protons, neutrinos, etc...
- Bosons: photons, Helium atoms, Higgs particle, etc...
- At low temperatures: inherently **quantum** behavior: e.g. **Bose-Einstein condensation**, superfluidity, quantized vortices, etc...
- Difficult to handle mathematically: usual approach **effective theories**.
- The connection between the original model and the effective theory is, in most cases, poorly understood.

## 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

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

- Main difficulty: dealing with the interactions.

## Known results

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- **Low density:** Lee-Huang-Yang formula

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

proved: [Lieb, Yngvason, 1998], [Yau, Yin, 2009], [Fournais, Solovej, 2020], [Basti, Cenatiempo, Schlein, 2021].

- **High density:** Hartree energy:

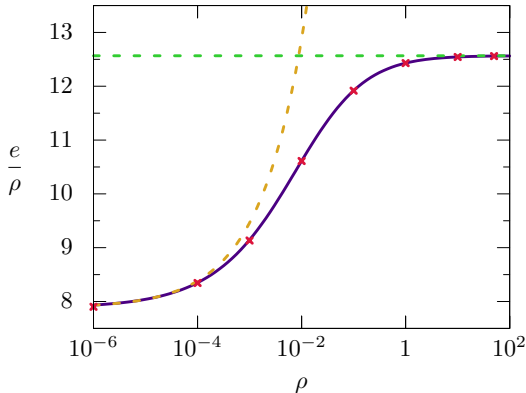
$$e_0 \sim \frac{\rho}{2} \int v$$

proved: [Lieb, 1963].

# The Simplified approach: proof of concept

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For  $v(x) = e^{-|x|}$ : Simplified approach, LHY, Hartree, Monte Carlo



## The Simplified approach

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- [Lieb, 1963], [Jauslin, 2023].
- 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,

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

## 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** (clustering property): 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: in general,

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

## Factorization assumption

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- **Lemma** [Lieb, 1963], [Jauslin, 2023]: Under the Factorization assumption and the consistency condition,

$$u_3(x - y) = u(x - y) + \frac{1}{V}(1 - u(x - y)) \int dz u(x - z)u(z - y) + O(V^{-2})$$

$$u_4(x - y) = u(x - y) + \frac{2}{V}(1 - u(x - y)) \int dz u(x - z)u(z - y) + O(V^{-2})$$

- With  $u(x) := 1 - g_2(0, x)$ .

## Big equation

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- In the thermodynamic limit,

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

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

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

- “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:**

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

This coincides with the **Hartree energy**.

- **Theorem 3:**

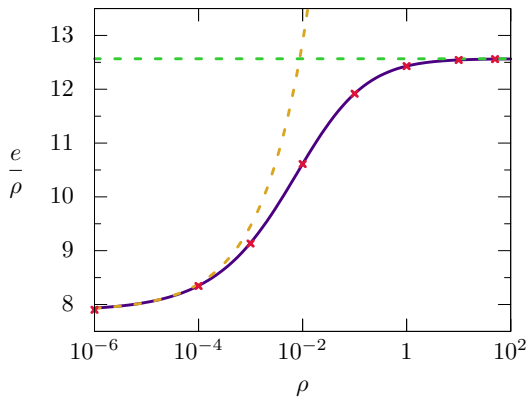
$$e = 2\pi\rho a \left( 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right)$$

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

# Energy

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



# Radial distribution function

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- Two-point correlation:

$$C_2(y - z) = \sum_{i,j} \langle \psi_0 | \delta(y - x_i) \delta(z - x_j) | \psi_0 \rangle.$$

- Radial distribution: spherical average and normalization:

$$G(r) := \frac{1}{\rho^2} \int \frac{dy}{4\pi r^2} \delta(|y| - r) C_2(y).$$

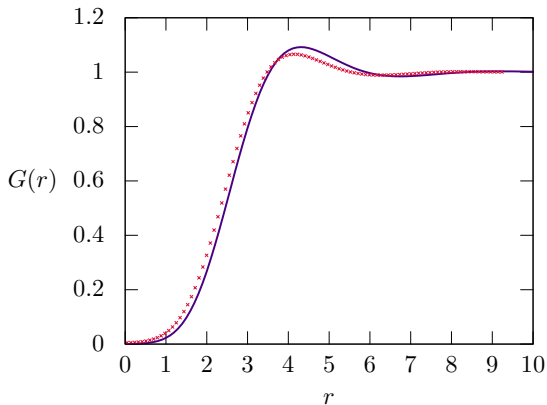
- Compute  $C_2$  using

$$C_2(x) = 2\rho \frac{\delta e_0}{\delta v(x)}.$$

# Radial distribution function

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

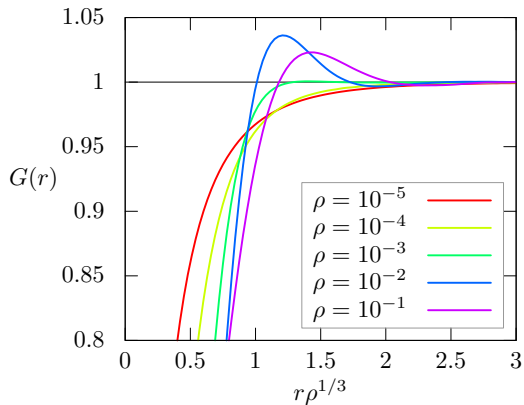




## Radial distribution function

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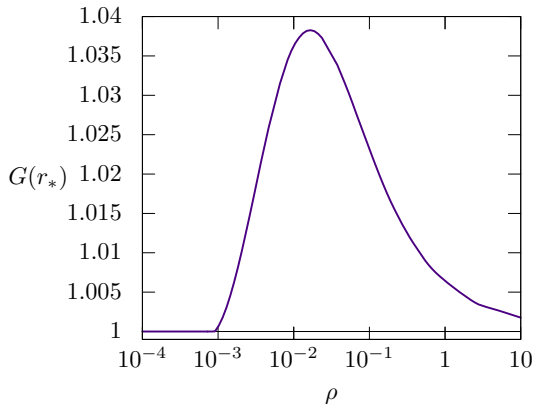
$$v(x) = 8e^{-|x|}, \rho = 10^{-5}-10^{-1}$$



## Radial distribution function

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



## Liquid behavior

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- 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**: **Liquid-like** behavior.

# Structure factor

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- **Structure factor:** Fourier transform of  $G$ :

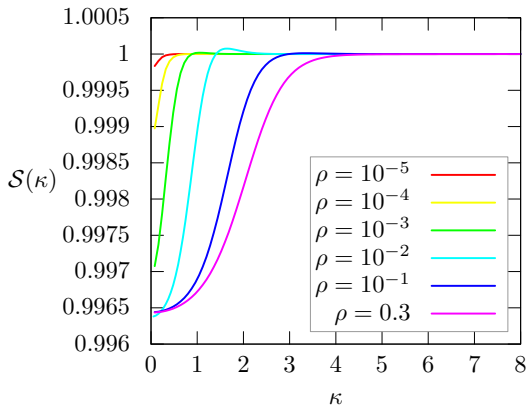
$$S(|k|) := 1 + \rho \int dx e^{ikx} (G(|x|) - 1).$$

- Directly observable in X-ray scattering experiments.
- Sharp peaks: order.
- Large deviation from 1: uniformity.

# Structure factor

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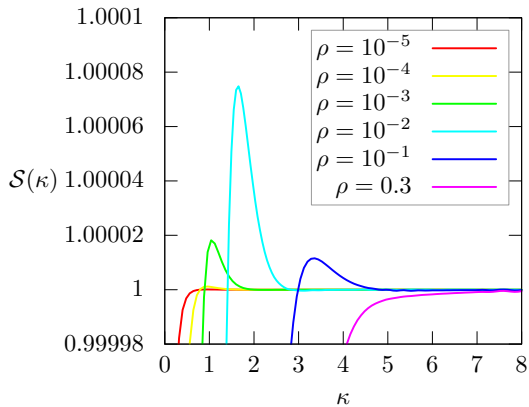
$$v(x) = 8e^{-|x|}, \rho = 10^{-5}-0.3$$



# Structure factor

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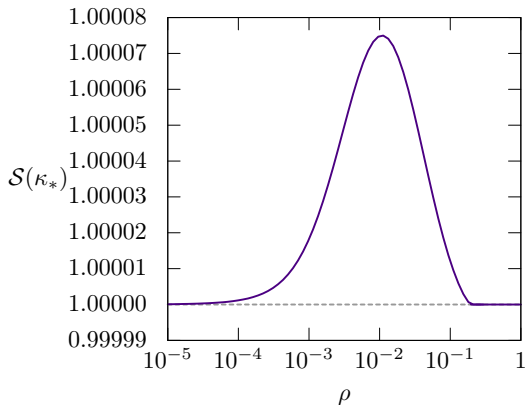
$$v(x) = 8e^{-|x|}, \rho = 10^{-5}-0.3$$



# Structure factor

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



## Liquid behavior

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- Sharpening of the peak: more order.
- Not Bragg peaks: **No** long range order.
- Larger deviation from 1: more uniform (not even close to hyperuniform).
- **Short-range order**: **Liquid**-like behavior.



## Critical densities

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- We have found two critical densities:  $\rho_* \approx 0.9 \times 10^{-3}$  and  $\rho_{**} \approx 0.2$ .
- The radial distribution function has a maximum only for  $\rho > \rho_*$ .
- The structure factor has a maximum only for  $\rho < \rho_{**}$ .

## Condensate fraction

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- Proportion of particles in the condensate state:

$$\eta := \frac{1}{N} \sum_i \langle \psi_0 | P_i | \psi_0 \rangle$$

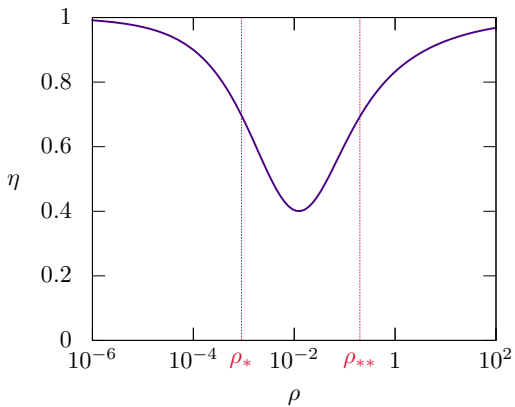
where  $P_i$  is the projector onto the constant state  $V^{-\frac{1}{2}}$ .

- $\eta > 0$  in thermodynamic limit: **Bose-Einstein condensation** (still not proved to occur).

# Condensate fraction

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$$v(x) = 8e^{-|x|};$$



## Summary and outlook

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- Using the **Simplified approach**, we were able to probe the repulsive Bose gas **beyond the dilute regime**.
- Evidence for **non-trivial behavior** at intermediate densities  $\rho_* < \rho < \rho_{**}$ : **short-range order**.
- Is there a phase transition?
- The intermediate density regime has not been studied much, due to the lack of tools to do so. As we have seen, there is non-trivial behavior there. This warrants further investigation, both theoretical and experimental.

## Open problems on the Simplified approach

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- Connect the Simplified approach to the many-Boson system: numerics suggests the prediction of the Simplified approach is an **upper bound**, for all densities.
- Understand the factorization assumption. It certainly does not hold exactly. Does it hold approximately, in some sense?
- There are still many questions about the Bose gas with hard core interactions. The Simplified approach is easily defined in the hard core case. Can it shed some light?