

Non-perturbative behavior of interacting Bosons at intermediate densities

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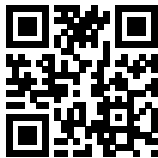
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Systems of interacting Bosons: What and why?

- Bosons are a **part of the natural world**:
 - ▶ Quantum particles are either **Fermions** or **Bosons** (in 3D).
 - ▶ Fermions: electrons, protons, neutrinos, etc...
 - ▶ Bosons: photons, Helium atoms, Higgs particle, etc...
- They exhibit **non-trivial physical behavior** at low temperatures: e.g. **Bose-Einstein condensation**, superfluidity, quantized vortices, etc...
- It is **difficult to handle mathematically**: for instance, Bose-Einstein condensation has **never been proved** in interacting models in the continuum at finite density.

Repulsive Bose gas

- 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**): ψ_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 theorems

- **Low density:** [Bogolyubov, 1947], [Lee, Huang, Yang, 1957]:

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

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

- [Lieb, 1963], [Jauslin, 2023].
- $\psi_0 \geq 0$, so it can be thought of as a probability distribution.
- g_n : **correlation functions** of $V^{-N}\psi_0$

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

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

$$g_n(x_1, \dots, x_n) = \prod_{1 \leq i < j \leq n} g_2(x_i - x_j), \quad u_n \in L_1(\mathbb{R}^3)$$

Equations of the simplified approach

- $u := 1 - g_2$:

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

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

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

- “Big” equation:

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

- Simple equation:

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

Theorems for the simple equation

- **Theorem 1:**

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

This coincides with the **Hartree energy**.

- **Theorem 2:**

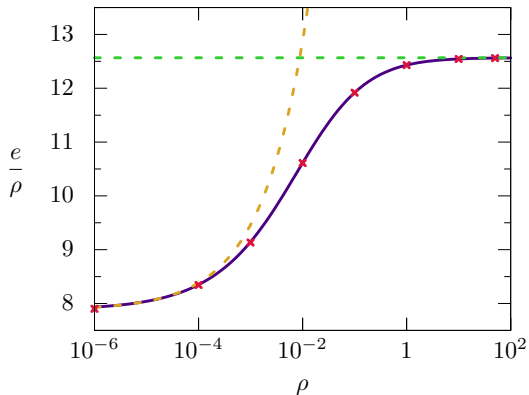
$$e = 2\pi\rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right)$$

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

- **Theorem 3:** The Simple equation predicts **Bose-Einstein condensation** at small densities.

Energy

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



Radial distribution function

- 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:

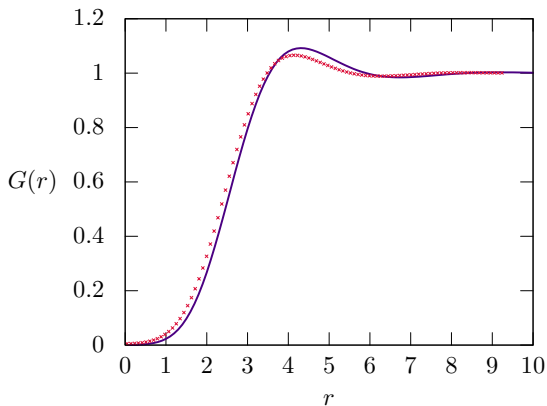
$$G(r) := \frac{1}{\rho^2} \int \frac{dy}{4\pi r^2} \delta(|y| - r) C_2(y).$$

- Compute C_2 using

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

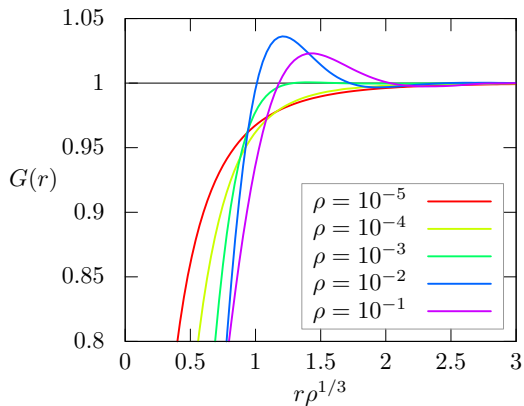
Radial distribution function

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



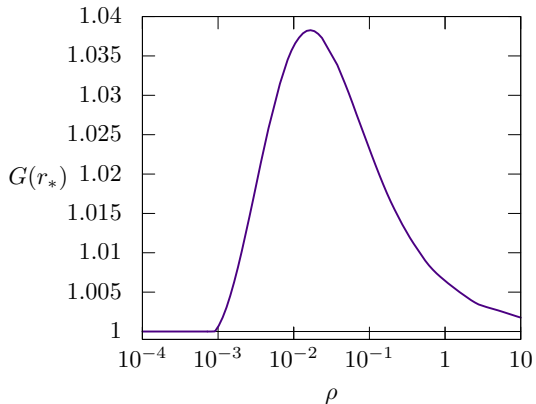
Radial distribution function

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



Radial distribution function

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



Structure factor

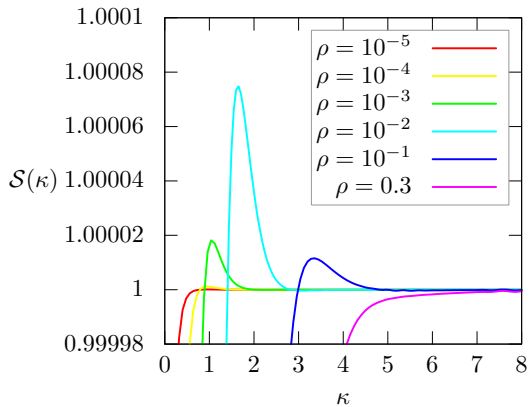
- **Structure factor:** Fourier transform of G :

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

- Directly observable in X-ray scattering experiments.
- Sharp peaks: order.

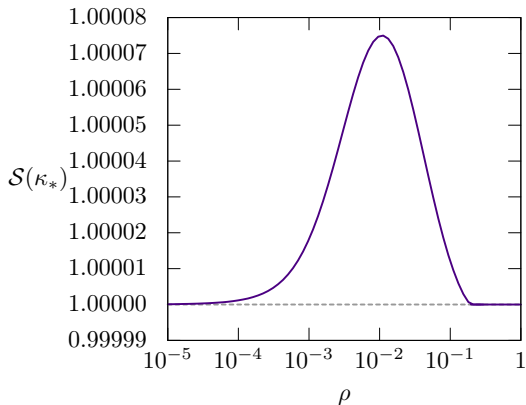
Structure factor

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



Structure factor

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



“Liquid” behavior

- 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**.
- Structure factor:
 - ▶ Sharpening of the peak.
 - ▶ Not Bragg peaks: **No** long range order: **Short-range order**.

Summary and outlook

- 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: **short-range order**.
- 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.