Non-perturbative behavior of interacting Bosons at intermediate densities

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Bosons

- 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

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

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

- Ground state (zero temperature): ψ_0, energy E_0.
- Observables in the thermodynamic limit: for instance, ground state energy per particle

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

- Main difficulty: dealing with the interactions.

Known results

- 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].

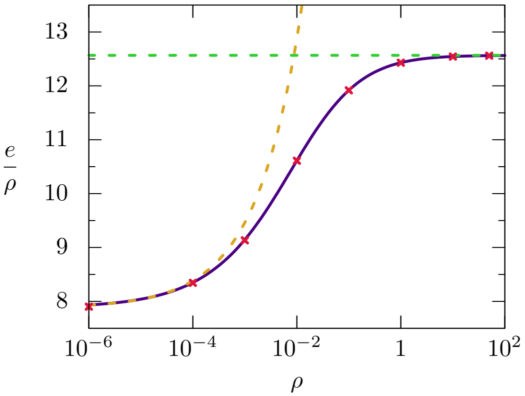
- High density: Hartree energy:

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

  proved: [Lieb, 1963].

The Simplified approach: proof of concept

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



The Simplified approach

- [Lieb, 1963], [Jauslin, 2023].
- Integrate $H_N\psi_0 = E_0\psi_0$:

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

- 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

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

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

- 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 $x_3, \cdots, x_N$:

$$-\frac{1}{2}(\Delta_x + \Delta_y)g_2(x,y) + \frac{N-2}{V}\int dz\ (v(x-z) + v(y-z))g_3(x,y,z)$$

$$+v(x-y)g_2(x,y) + \frac{(N-2)(N-3)}{2V^2}\int dzdt\ v(z-t)g_4(x,y,z,t) = E_0 g_2(x,y)$$

- Infinite hierarchy of equations.

Factorization assumption

- Factorization assumption (clustering property): for $n = 3, 4$,

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

- 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

- **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

- In the thermodynamic limit,

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

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

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

- "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 $v(x) \geqslant 0$ and $v \in L_1 \cap L_2(\mathbb{R}^3)$, then the simple equation has an integrable solution (proved constructively), with $0 \leqslant u \leqslant 1$.

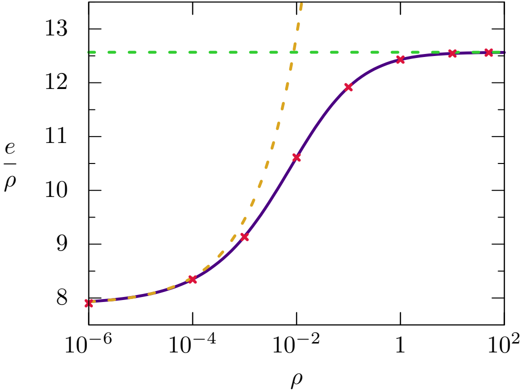
Energy for the simple equation

- **Theorem 2**:
$$\frac{e}{\rho} \underset{\rho\to\infty}{\longrightarrow} \frac{1}{2}\int dx\ v(x).$$
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

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

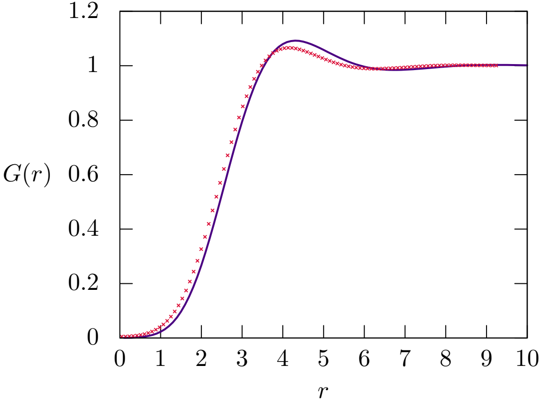
$$G(r) := \frac{1}{\rho^2}\int \frac{dy}{4\pi r^2}\;\delta(|y|-r)C_2(y).$$

- Compute C_2 using

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

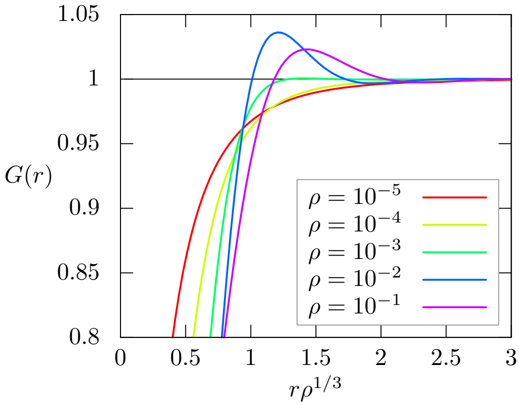
Radial distribution function

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



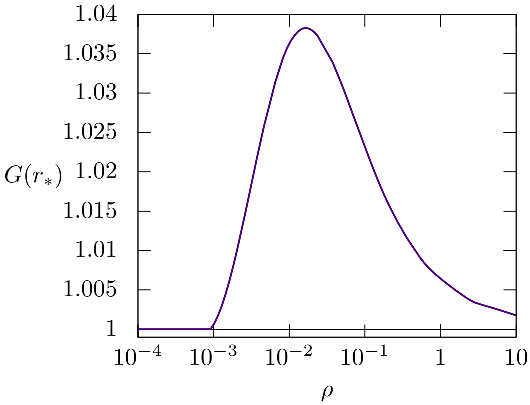
Radial distribution function

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



Radial distribution function

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



Liquid behavior

- 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

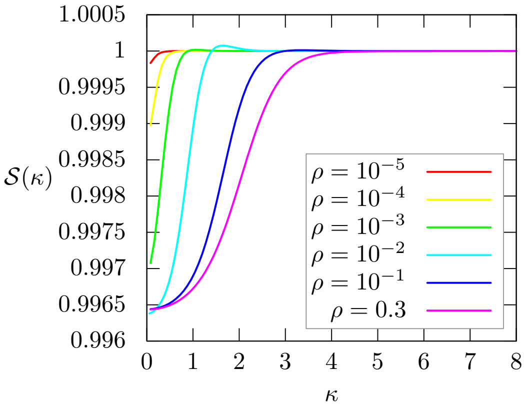
- Structure factor: Fourier transform of G:

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

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

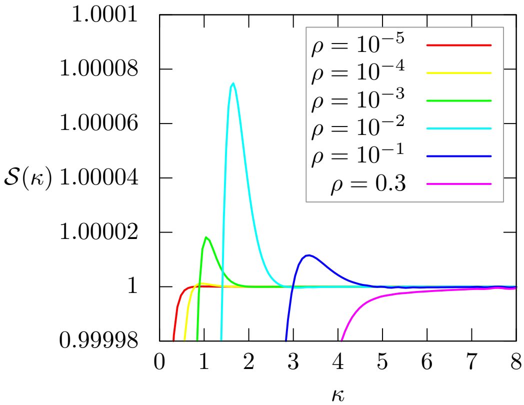
Structure factor

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



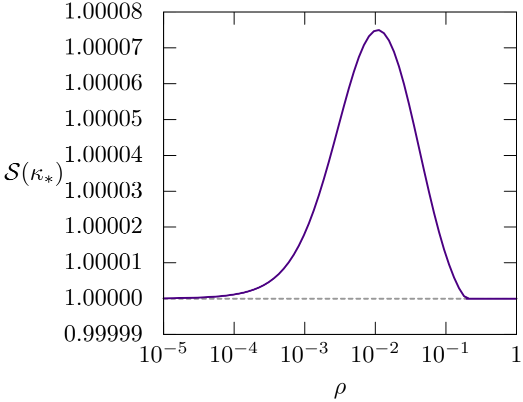
Structure factor

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



Structure factor

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



Liquid behavior

- 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

- 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

- Proportion of particles in the condensate state:

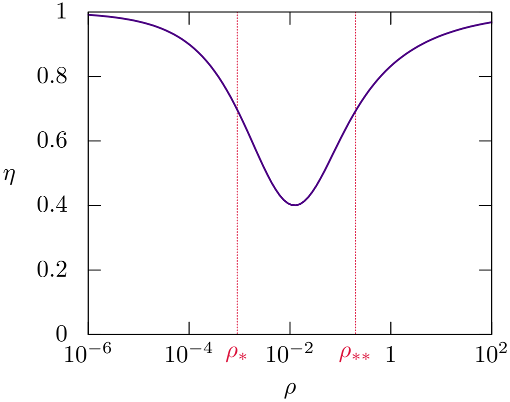
$$\eta := \frac{1}{N} \sum_i \langle \psi_0 | P_i | \psi_0 \rangle$$

  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

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



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 $\rho_* < \rho < \rho_{**}$: 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

- 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?