The Simplified approach to the Bose gas

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Congratulations, Jakob!

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Motivation

- 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

- 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

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

The Simplified approach

- [Lieb, 1963], [Jauslin, 2025].
- Integrate $H_N\psi_0 = E_0\psi_0$:

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

- Therefore,

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

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: 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: 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

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

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

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

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

- "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**: If $v(x) \geqslant 0$ 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 $0 \leqslant u \leqslant 1$.

Comparison to the many-body Bose gas: notation

- 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

- **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

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

The Ground state energy

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

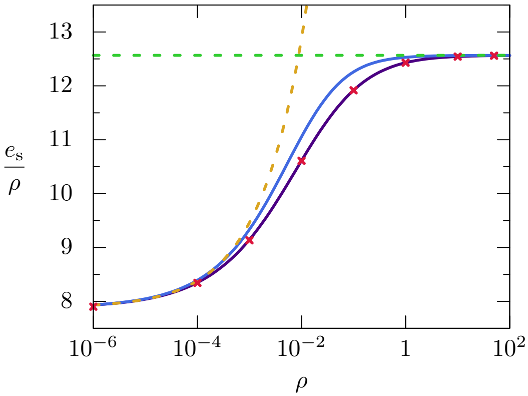
$$\frac{e_0}{\rho} \underset{\rho\to\infty}{\longrightarrow} \frac{\rho}{2}\int dx\ v(x)$$

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

$$\frac{e_{\mathrm{s}}}{\rho} \underset{\rho\to\infty}{\longrightarrow} \frac{1}{2}\int dx\ v(x).$$

The Ground state energy

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



Condensate fraction

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

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

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

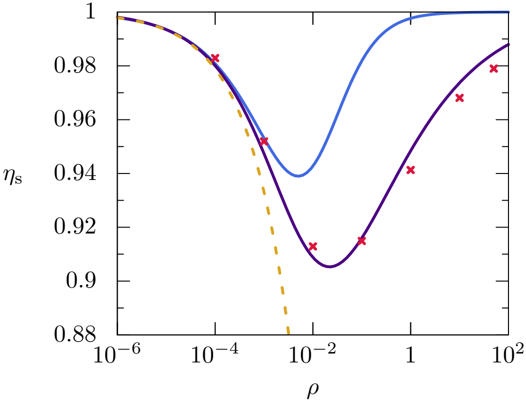
$$\eta_0 = 1 - \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}} + o(\sqrt{\rho a^3})$$

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

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

Condensate fraction

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



Two-point correlation

- $$C_0^{(2)}(y-z) := \lim_{\substack{V,N\to\infty\\ \frac{N}{V}=\rho}} \sum_{i,j} \langle\psi_0|\,\delta(y-x_i)\delta(z-x_j)\,|\psi_0\rangle\,.$$
- **Conjecture**: [Lee, Huang, Yang, 1957] As $\sqrt{\rho a}|x|\to\infty$,
$$\frac{1}{\rho^2}C_0^{(2)}(x)-1\sim\frac{\frac{16a}{\pi^3\rho}}{|x|^4}$$
- **Theorem**: For the Simple equation, if $(1+|x|^6)v\in L_1$, then
$$\frac{1}{\rho^2}C_{\mathrm{s}}^{(2)}(x)-1\sim\frac{c(\rho)}{|x|^4}+r(x)$$
with $|x|^4 r\in L_2\cap L_\infty$.

Universal Tan relations

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

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

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

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

Universal Tan relations

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

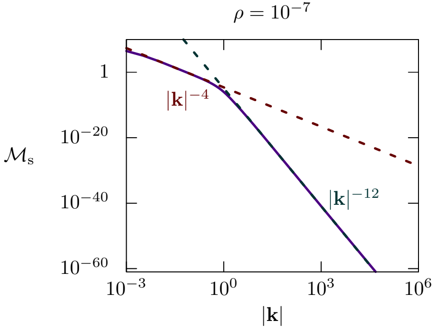
$$\mathcal{M}_0(k) \sim \frac{16\pi^2 \rho a^2}{|k|^4}$$

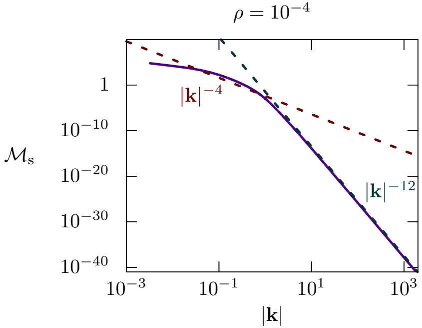
- The Simple equation predicts that the Tan relation holds in the regime

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

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

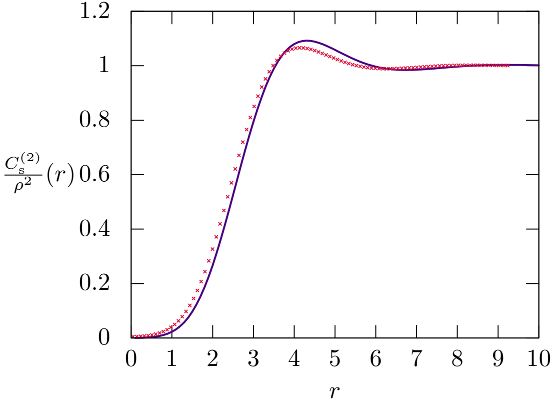
Breakdown of the Universal Tan relations





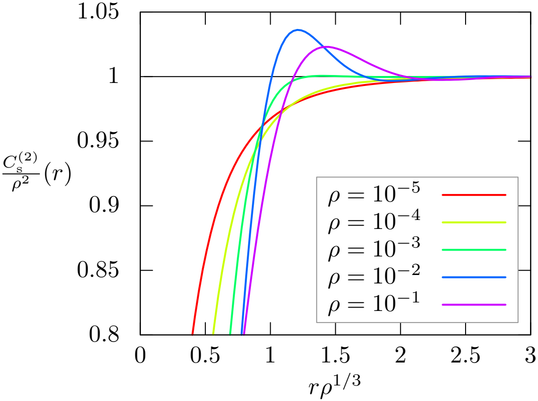
Two-point correlation function at intermediate density

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



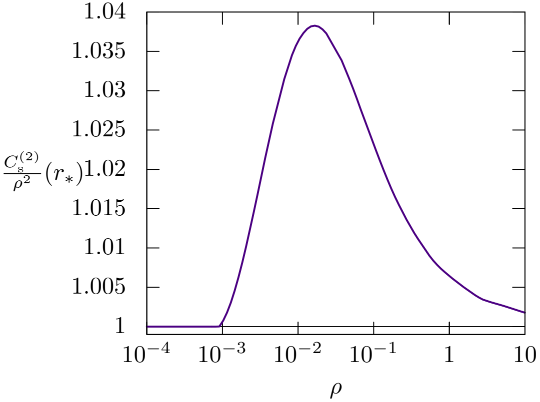
Two-point correlation function at intermediate density

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



Two-point correlation function at intermediate density

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

Summary

- 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

- **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

- **Mathematical Physics**
  - Control the factorization assumption.
  - Construct a trial state for the many-body Bose gas. Natural choice: Bijl-Dingle-Jastrow function

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

    where u is the solution to the Simple equation.