

A new approach to the Mathematics of the Bose gas

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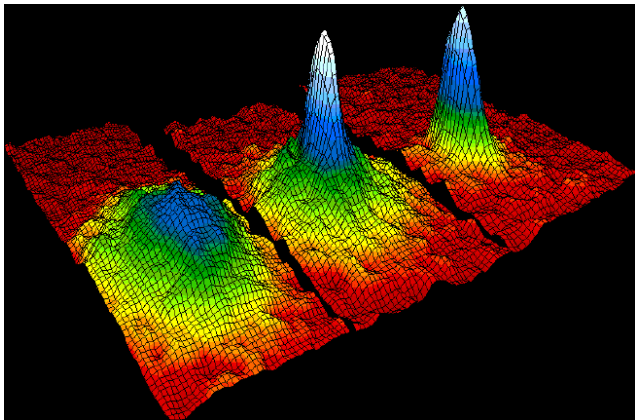
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Bose-Einstein condensation

- System of many Bosons, e.g. **Helium** atoms, **Rubidium** atoms, etc...
- **Bose-Einstein condensate**: most particles are in the same quantum state.
- Related to the phenomena of **superfluidity** and **superconductivity**.
- Predicted theoretically in **1924-1925**, experimentally observed in **1995**.
- Mathematical understanding: still **no proof** of the existence of a condensate (at finite density, in the presence of interactions and in the continuum).

Bose-Einstein condensation



Repulsive Bose gas

- N -particle quantum state in a volume V :

$$\psi_N(x_1, \dots, x_N) \in L^2_{\text{symmetric}}((V\mathbb{T}^3)^N)$$

- $|\psi|^2$: probability distribution on the positions of the N particles.
- Hamiltonian operator acting on ψ :

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

$$v(r) \geq 0, \hat{v}(k) \geq 0 \text{ and } v \in L_1(\mathbb{R}^3).$$

Energy and condensate fraction

- Ground state: ψ_0 , energy E_0 :

$$H_N \psi_0 = E_0 \psi_0$$

- In the **thermodynamic limit**:

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

- Condensate fraction: proportion of particles in the Bose-Einstein condensate: in the **thermodynamic limit**:

$$\eta_0 := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{1}{N} \langle \psi_0 | \sum_{i=1}^N \int \frac{dx_i}{V} | \psi_0 \rangle.$$

Low density conjectures

- Bogolubov theory: **approximation scheme** [Bogolubov, 1947].
- Predictions [Lee, Huang, Yang, 1957]:

▶ Energy:

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

▶ Condensate fraction:

$$1 - \eta_0 \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

Low density conjectures

- Energy asymptotics: **proved**: [Lieb, Yngvason, 1998], [Yau, Yin, 2009], [Fournais, Solovej, 2019]
- Condensate fraction: **still open** in the thermodynamic limit. (No proof of Bose-Einstein condensation.)
- There are proofs of condensation in the ultra-dilute (Gross-Pitaevskii) regime: [Lieb, Seiringer, 2002], [Boccato, Brennecke, Cenatiempo, Schlein, 2018].
- There is also a proof of condensation for a **lattice** Bose gas [Kennedy, Lieb, Shastry, 1988].

High density conjectures

- [Bogolubov, 1947]:

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

- **Proved** in [Lieb, 1963].
- Condensate fraction: mean field regime: $\eta_0 \rightarrow 1$. (No proof of Bose-Einstein condensation at any density.)

Simple equation

- Simple equation

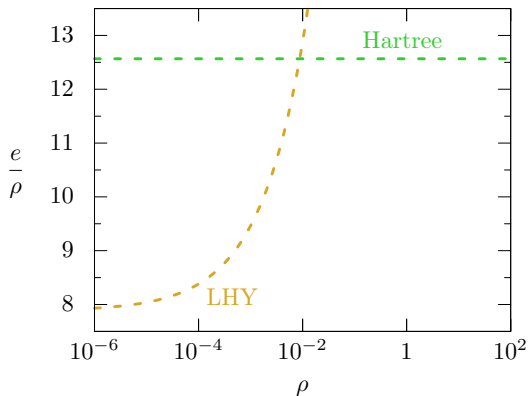
$$-\Delta u(x) = (1 - u(x))v(x) - 4eu(x) + 2e\rho u * u(x)$$

$$e = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

- $\rho > 0$: density, $v(x) \geq 0$, $v \in L_1(\mathbb{R}^3)$.
- **Non-linear** and **non-local** partial differential equation.

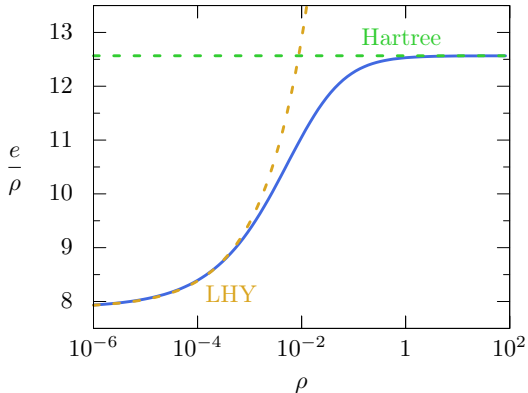
Energy as a function of density

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



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Derivation of the equation

- [Lieb, 1963].
- 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,

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

Derivation of the equation

- Thus,

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

- $\psi_0 \geq 0$, so it can be thought of as a probability distribution.
- g_n : **correlation functions** of ψ_0

$$g_n(x_1, \dots, x_n) := \frac{V^n \int dx_{n+1} \cdots dx_N \psi_0(x_1, \dots, x_N)}{\int dx_1 \cdots dx_N \psi_0(x_1, \dots, x_N)}$$

Hierarchy

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

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

- Factorization **assumption**:

$$g_3(x_1, x_2, x_3) = g_2(x_1, x_2)g_2(x_1, x_3)g_2(x_2, x_3)$$

$$g_4(x_1, x_2, x_3, x_4) = \prod_{i < j} (g_2(x_i, x_j) + O(V^{-1}))$$

Big equation

- In the thermodynamic limit, if $u(x) := 1 - g_2(0, x)$,

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

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

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

- “Big” equation:

$$L \approx u * u * S.$$

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 $v(x) \geq 0$ 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

- **Theorem 2:**

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

This coincides with the **Hartree energy**.

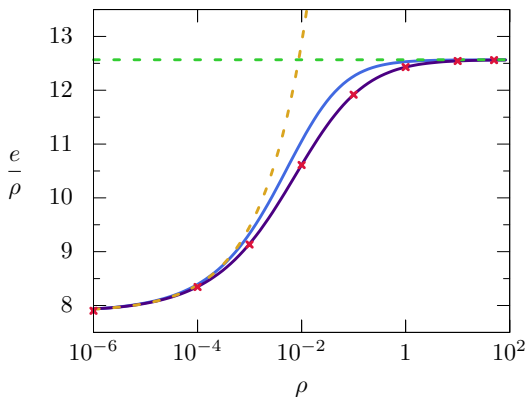
- **Theorem 3:**

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

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

Energy

$v(x) = e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Condensate fraction

- Add a parameter μ to the Hamiltonian:

$$H_N(\mu) := -\frac{1}{2} \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j) - \mu \sum_{i=1}^N \int \frac{dx_i}{V}.$$

- Projection onto condensate wavefunction: $\sum_i \int \frac{dx_i}{V}$.
- Condensate fraction:

$$\eta_0 := \frac{1}{N} \langle \psi_0 | \sum_{i=1}^N \int \frac{dx_i}{V} | \psi_0 \rangle = -\frac{1}{N} \partial_\mu \langle \psi_0 | H_N(\mu) | \psi_0 \rangle |_{\mu=0} \equiv -\partial_\mu e_0(\mu) |_{\mu=0}$$

Condensate fraction

- **Theorem 4:** For the **simple equation**, as $\rho \rightarrow 0$

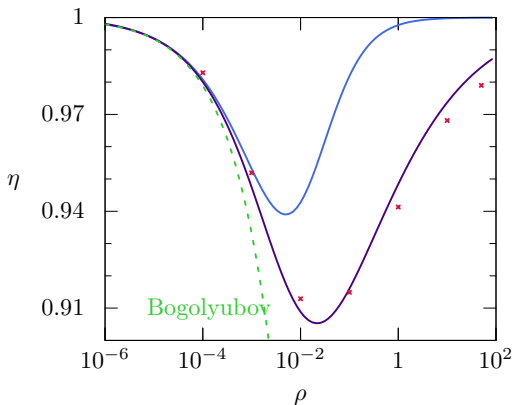
$$1 - \eta \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

which coincides with **Bogolubov's prediction**.

- In particular **there is Bose-Einstein condensation** for the simple equation.

Condensate fraction

$v(x) = e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Conclusions and outlook

- Two **effective equations**: the **big equation** and the **simple equation**, which are **non-linear 1-particle equations**.
- Reproduce the known results for both **small and large densities**.
- Their derivation is **different from Bogolubov theory**, so they may give new insights onto studying the Bose gas in these asymptotic regimes.
- The **big equation** is **quantitatively accurate** at intermediate densities.
- This opens up the possibility of studying the physics of the **Bose gas at intermediate densities**.

Open problems and next steps

- Analysis of the **big equation**: everything is still open.
 - ▶ Main tool: **Newton algorithm**, which works numerically.
 - ▶ There is a family of **intermediate equations** that extrapolate between the **simple** and **big** equations.
- Relate these equations back to the **many-body Bose gas**.
 - ▶ **Upper bound** for the ground state energy, using a **Bijl function** as a test function.
 - ▶ **Lee-Huang Yang formula** by studying the low-density properties of the **Bijl function**.
 - ▶ Extend the proof to the **condensate fraction**.