An effective equation to study Bose gases at all densities

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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 (flow with zero viscocity) and superconductivity (currents with zero resistance).
- 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).

Repulsive Bose gas

- Potential: $v(r) \geqslant 0$ and $v \in L_1(\mathbb{R}^3)$, Hamiltonian:

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

- Ground state: ψ_0, energy E_0.
- Observables in the thermodynamic limit: ground state energy per particle and condensate fraction: P_i: projection onto condensate state

$$e_0 := \lim_{\substack{V,N\to\infty \\ \frac{N}{V}=\rho}} \frac{E_0}{N}, \quad \eta_0 := \lim_{\substack{V,N\to\infty \\ \frac{N}{V}=\rho}} \frac{1}{N}\sum_{i=1}^{N} \langle\psi_0|\, P_i\, |\psi_0\rangle\,.$$

Low density

- Bogolyubov theory: approximation scheme that reduces the problem to an effective 1-particle problem.
- 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

- Energy asymptotics: proved: [Lieb, Yngvason, 1998], [Yau, Yin, 2009], [Fournais, Solovej, 2020].
- Condensate fraction: still open in the theormodynamic limit, but there are proofs of condensation in the Gross-Pitaevskii regime (ultra-dilute): [Lieb, Seiringer, 2002], [Boccato, Brennecke, Cenatiempo, Schlein, 2018].

High density

- [Bogolyubov, 1947]: if $\hat{v} \geqslant 0$.

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

  Hartree (mean field) energy.

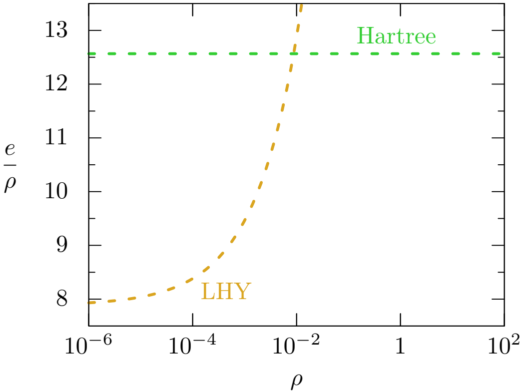
- Proved in [Lieb, 1963].
- Condensate fraction

$$\eta \to 1$$

  open.

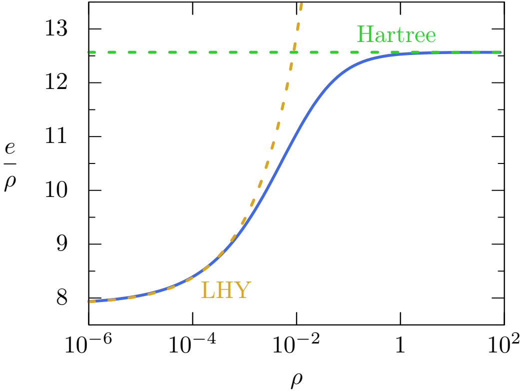
Energy as a function of density

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



Energy as a function of density

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



Derivation of the equation

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

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

- Therefore,

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

Derivation of the equation

- Thus,

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

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

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

Hierarchy

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

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

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

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

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

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

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

- "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**:

$$\frac{e}{\rho} \underset{\rho\to\infty}{\longrightarrow} \frac{1}{2}\int dx\ v(x)$$

(note that there is no condition that $\hat{v} \geqslant 0$). This coincides with the Hartree energy.

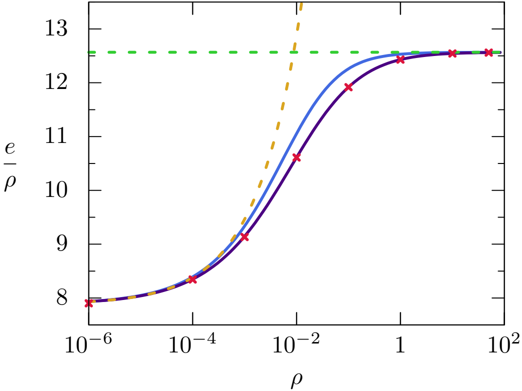
- **Theorem 3**:

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

This coincides with the Lee-Huang-Yang prediction.

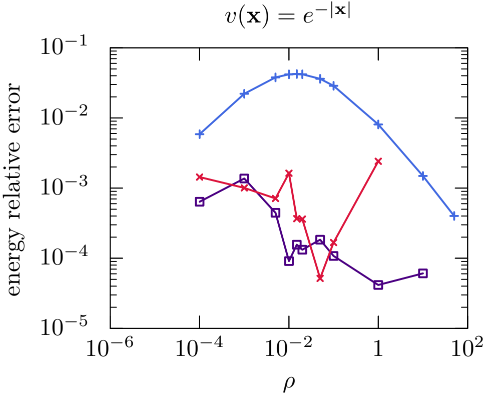
Energy

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



Energy

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



Condensate fraction

- Add a parameter μ to the Hamiltonian:

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

- Projection onto condensate wavefunction: P_i.
- Condensate fraction:

$$\eta_0 := \frac{1}{N}\langle\psi_0|\sum_{i=1}^{N} P_i|\psi_0\rangle = -\frac{1}{N}\partial_\mu\langle\psi_0|H_N(\mu)|\psi_0\rangle|_{\mu_0} \equiv -\partial_\mu e_0(\mu)|_{\mu=0}$$

Condensate fraction

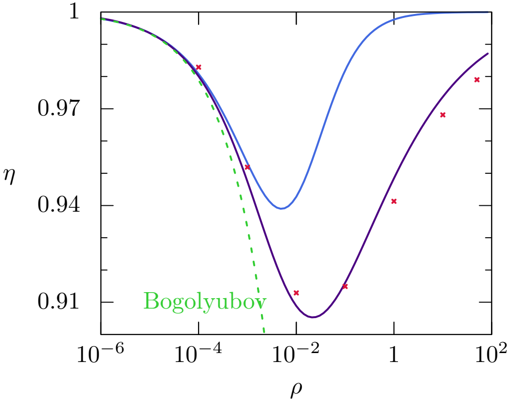
- **Theorem 4**: For the simple equation, as $\rho \to 0$

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

which coincides with Bogolyubov's prediction.

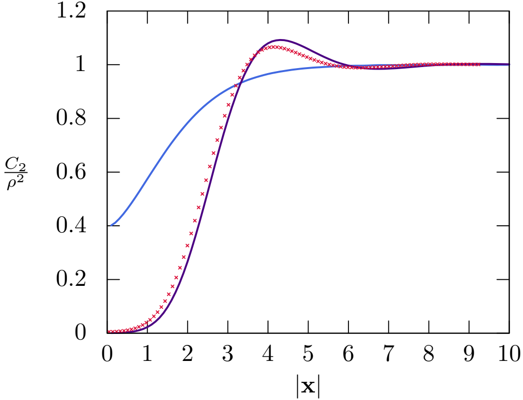
Condensate fraction

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



Two point correlation function

$v(x) = 16e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Summary 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 Bogolyubov 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

- Uniqueness of the solution of the simple equation (done for small and large ρ).

- LHY as an upper bound at low density using the simple equation to construct an Ansatz.

- Existence (and uniqueness) of the solution of the big equation.

The uniqueness problem

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

- Change the point of view: fix $e > 0$, and compute ρ and u.
- Iteration: $u_0 = 0$,

$$(-\Delta + 4e + v)u_n = v + 2e\rho_{n-1}u_{n-1} * u_{n-1}, \quad \rho_n := \frac{2e}{\int dx\ (1-u_n(x))v(x)}.$$

The uniqueness problem

- **Lemma**: $u_n(x)$ is an increasing sequence, and is bounded $u_n(x) \leqslant 1$. It converges to a function u, which is the unique integrable solution of the equation with e fixed.
- **Lemma**: $e \mapsto \rho(e)$ is continuous, and $\rho(0) = 0$ and $\rho(\infty) = \infty$, which allows us to compute solutions for the problem at fixed ρ.
- We thus have a restricted notion of uniqueness. The full uniqueness would follow from a proof that $e \mapsto \rho(r)$ is monotone increasing (which must be true for the physics to make sense).

Upper bound at low density

- [Yau, Yin, 2009]: proof for weak, smooth, rapidly decaying potentials.
- [Basti, Cenatiempo, Schlein, 2021]: extended for L_3 (and compactly supported) potentials (excludes hard-core interactions).
- Simple Equation: our analysis holds for the hard-core, so if one could find a good Ansatz from it, one might get an upper bound for the energy in this case.
- Idea for Ansatz? (Jastrow, Dyson-Jastrow?).

Upper bound at low density: Jastrow function

- Idea:

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

- Why this: $\rho \ll 1$, and if $\rho \|u\|_1 \ll 1$,

$$g_2 \sim 1 - u.$$

- Again, if $\rho \|u\|_1 \ll 1$, we would be able to compute the energy of ψ using a cluster expansion!
- However, $\|u\|_1 = \frac{1}{\rho}$!

Existence for the Big Equation

- Numerical method: Newton algorithm.
- For the existence of a solution, it would suffice to prove that the Newton algorithm has a Basin of attraction. (Kantorovich-like theorem?)
- Such a result, applied to the Simple Equation, would imply the uniqueness of a solution (provided we have convergence in an appropriate norm).