# Analysis of a non-linear, non-local PDE to study Bose gases at all densities

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# Simple equation

- Simple equation

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

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

- $\rho > 0$, $v(x) \geqslant 0$, $v \in L_1(\mathbb{R}^3)$.
- Non-linear and non-local partial differential equation.
- Effective equation for the ground state of a Bose gas.

# 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

- $N$-particle quantum state in a volume $V$:

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

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

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

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

# Energy and condensate fraction

- Ground state: $\psi_0$, energy $E_0$:

$$H_N\psi_0 = E_0\psi_0$$

- In the thermodynamic limit:

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

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

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

# Low density conjectures

- Bogolyubov theory: approximation scheme [Bogolyubov, 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, 2020].
- 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

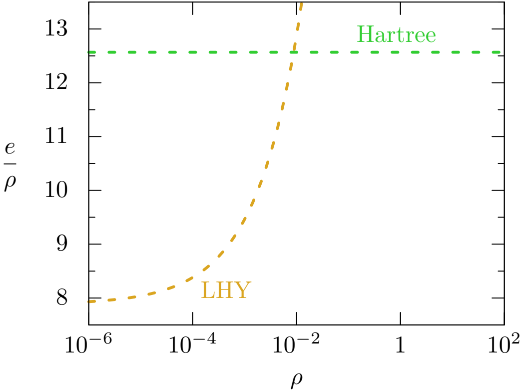
- [Bogolyubov, 1947]:

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

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

# Energy as a function of density for the Simple equation

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



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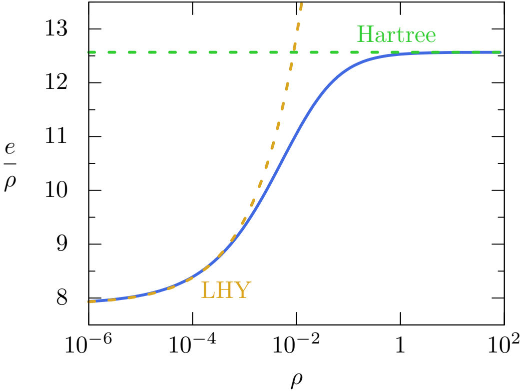


# Effective equations

- Boltzmann equation: $N$ classical hard particles with an infinitely small radius (dilute limit) [Lanford, 1976].
- Thomas-Fermi theory: $Z$ electrons orbiting a nucleus in the $Z \to \infty$ limit [Lieb, Simon, 1973].
- Hartree-Fock equation: dynamics of many Fermions in the weakly-interacting limit [Benedikter, Porta, Schlein, 2015].
- Hartree-Fock-Bogolyubov equation: dynamics of many Bosons in the weakly-interacting limit [Bach, Breteaux, Chen, Fröhlich, Sigal, 2016].

# 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 $\psi_0$

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

# 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:

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

# 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 $0 \leqslant u \leqslant 1$.

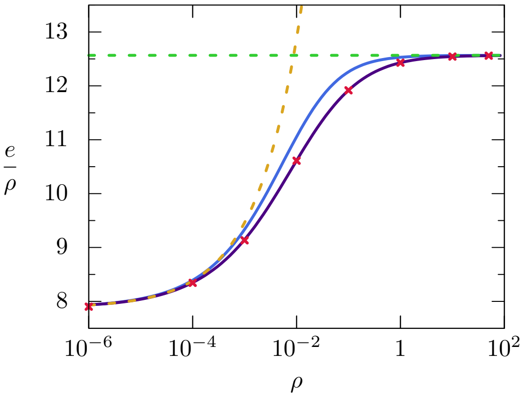
# Energy for the simple equation

- **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

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



# Condensate fraction

- Add a parameter $\mu$ to the Hamiltonian:

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

- 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 $\rho \to 0$

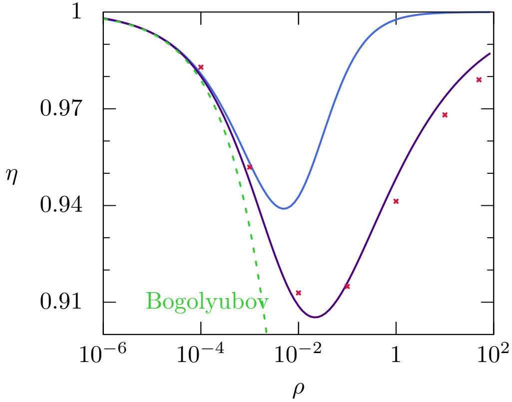
$$1 - \eta \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

  which coincides with Bogolyubov'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 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 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.