An effective equation to study Bose gasses at all densities

Ian Jauslin

joint with Eric A. Carlen, Markus Holzmann, Elliott H. Lieb

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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 viscosity) 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: \( v(r) \geq 0 \) and \( v \in L^1(\mathbb{R}^3) \), Hamiltonian:

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

- Ground state: \( \psi_0 \), energy \( E_0 \).

- Observables in the thermodynamic limit: ground state energy per particle and condensate fraction: \( P_i \): projection onto condensate state

\[
e_0 := \lim_{V,N \to \infty} \frac{E_0}{N}, \quad \eta_0 := \lim_{V,N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \langle \psi_0 | P_i | \psi_0 \rangle.
\]
Low density

• Bogolubov 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 thermodynamic limit, but there are proofs of condensation in the Gross-Pitaevskii regime (ultra-dilute): [Lieb, Seiringer, 2002], [Boccato, Brennecke, Cenatiempo, Schlein, 2018].

• In Gross-Pitaevskii limit, can also compute excitation spectrum: [Boccato, Brennecke, Cenatiempo, Schlein, 2019].
High density

- [Bogolubov, 1947]: if $\hat{v} \geq 0$.

\[ e_0 \sim \frac{\rho}{2} \int v \]

- Proved in [Lieb, 1963].

- The ultra-concentrated limit is the Hartree regime, in which the excitation spectrum can also be computed: [Seiringer, 2011].
Energy as a function of density

For $v(x) = e^{-|x|}$:
Energy as a function of density

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

![Graph showing the energy as a function of density for different potentials, labeled as LHY and Hartree.](image)
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 \( V^{-N} \psi_0 \)

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

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

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

\[
+ v(x - y)g_2(x, y) + \frac{(N - 2)(N - 3)}{2V^2} \int dzt \ v(z - t)g_4(x, y, z, t) = E_0g_2(x, y)
\]

- Factorization assumption:

\[
g_3(x_1, x_2, x_3) = g_2(x_1, x_2)g_2(x_1, x_3)g_2(x_2, x_3)
\]

\[
g_4(x_1, x_2, x_3, x_4) = \prod_{i<j}(g_2(x_i, x_j) + O(V^{-1}))
\]
• In the thermodynamic limit, if $u(x) := 1 - g_2(0, x)$,

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

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

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

• “Big” equation:

$$L \approx u \ast u \ast S.$$
• Further approximate $S(x) \approx \frac{2e}{\rho} \delta(x)$ and $u \ll 1$.

• Simple equation

\[-\Delta u(x) = (1 - u(x))v(x) - 4eu(x) + 2e\rho u \ast u(x)\]

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

• **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:**
  \[
  e \rightarrow \frac{1}{\rho} \rightarrow_{\rho \rightarrow \infty} \frac{1}{2} \int dx \, v(x)
  \]
  (note that there is no condition that \( \hat{v} \geq 0 \)). 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
$v(x) = e^{-|x|}$, Blue: simple equation; red: Jastrow; purple: big equation

$\rho_v(x) = e^{-|x|}$

![Graph showing energy relative error](image)
• Add a parameter $\mu$ to the Hamiltonian:

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

• Projection onto condensate wavefunction: $P_i$.

• Condensate fraction:

$$\eta_0 := \frac{1}{N} \langle \psi_0 | \sum_{i=1}^{N} P_i | \psi_0 \rangle = -\frac{1}{N} \partial_\mu \langle \psi_0 | H_N(\mu) | \psi_0 \rangle |_{\mu=0} \equiv -\partial_\mu e_0(\mu)|_{\mu=0}$$
• **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 Bogolubov’s prediction.
Condensate fraction

\[ v(x) = e^{-|x|}, \text{ Blue: simple equation; purple: big equation; red: Monte Carlo} \]
Linear correlation function

\[ v(x) = 16e^{-|x|}, \quad \text{Blue: simple equation; purple: big equation; red: Jastrow} \]
Limitations of the simple and big equations

- Only works at high densities for \( \hat{v} \geq 0 \).
- Less accurate for large potentials: for \( v(x) = 16e^{-|x|} \),

![Graph 1](image1.png)

![Graph 2](image2.png)
Conclusions and outlooks

• 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

• Analysis of the simple equation: Monotonicity of $e(\rho)$, and convexity of $\rho e(\rho)$. (So far, we have proofs for small and large $\rho$.) Similarly, prove that $0 \leq \eta \leq 1$. (We have a proof for small $\rho$.)

• Analysis of the big equation: everything is still open.

• Relate these equations back to the many-body Bose gas.